"Supporting Information for"

DFT Mechanistic Investigation into the Phenol Dearomatization Mediated by an Iodide(III) reagent

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Content

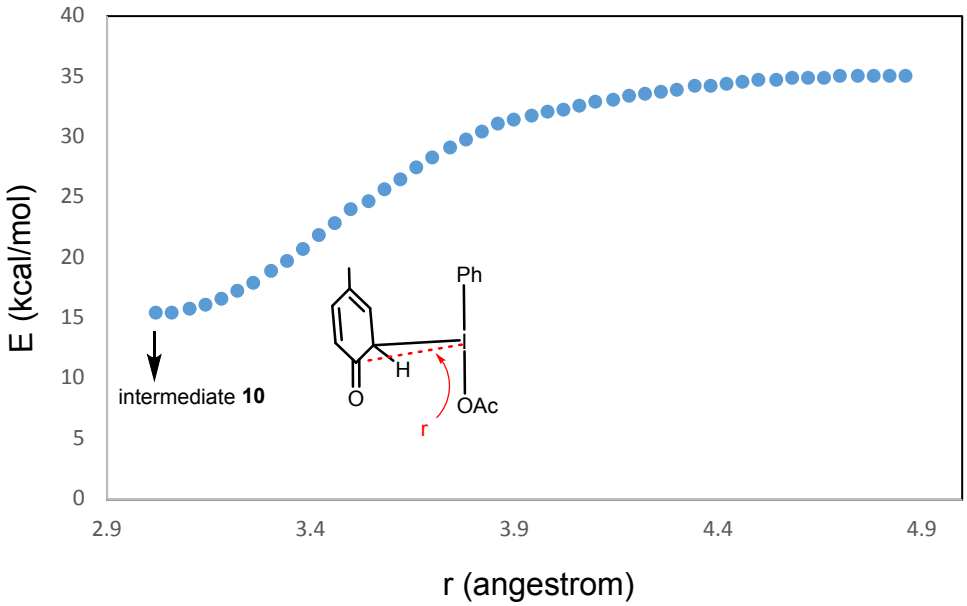

Fig. S1 Relaxed potential energy surface scan starting from intermediate **10** calculated at M06-2X-SMD/BS1 level. The presence of the OAc^- in structure **10** causes it to be unreactive toward the redox process via the dissociative mechanism. Indeed, this anion increases the nucleophilicity of the iodine(III) center, not allowing the redox to be accessible directly from **10**. The potential energy surface scan for formation of phenoxenium ion from **10** was found to be endergonic (more than 35 kcal/mol).

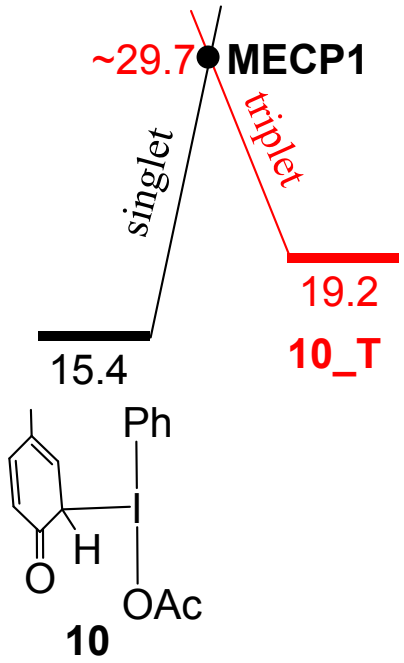

Fig. S2 Gibbs free energy profile (kcal/mol) for conversion of **10** on the singlet surface to that on the triplet by passing through **MECP1** calculated at the M06-2X-SMD/BS2//M06-2X-SMD/BS1 level.

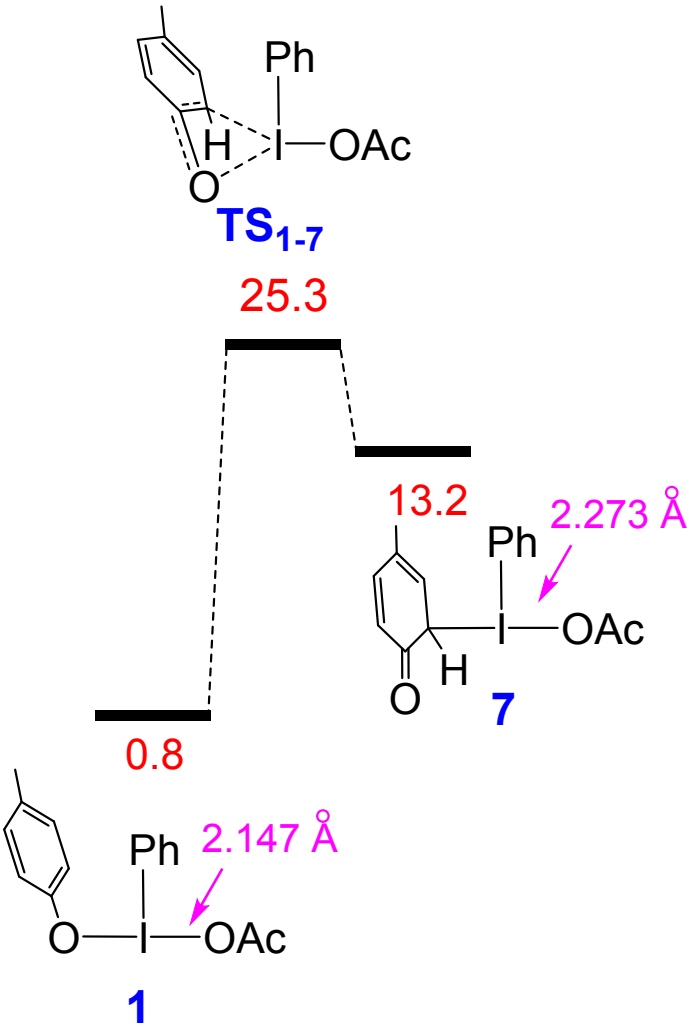

Fig. S3 Gibbs free energy profile (kcal/mol) for interconversion of **1** to **7.**

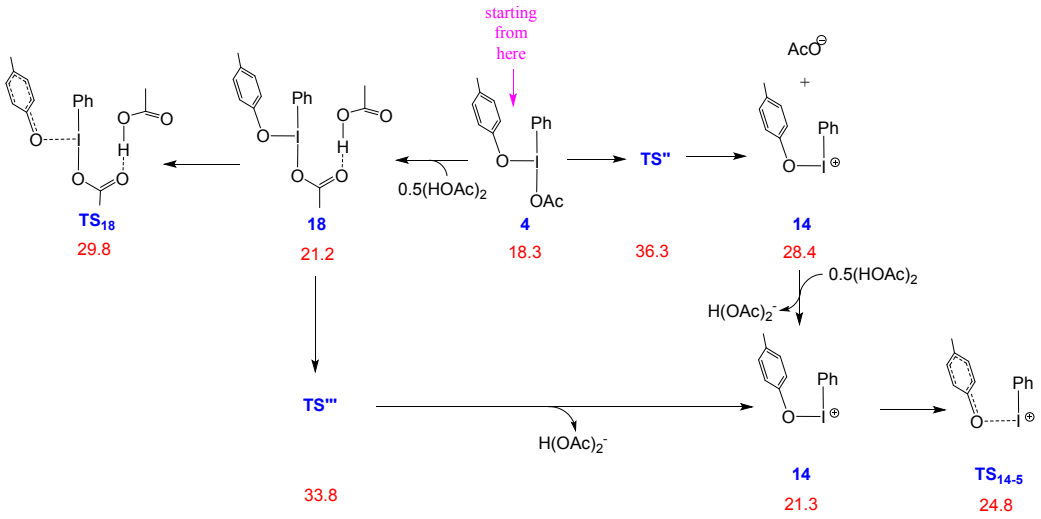

Fig. S4 Calculated mechanism of phenol dearomatization starting from **4** via different variants occurring through vital transition structures **TS_{18}**, **TS″** and **TS‴**. All these calculations show that **4** is much less reactive than **10** for phenol dearomatization. Free energies are given in kcal/mol.

Other methodologies for calculating the Gibbs free energies.

For the sake of comparison, we also applied other methodologies for calculation of free energies. The methodology given in eq. S1 was applied for all the energy profiles. In eq. S1, $E^{M06-2X-SMD/BS2}$ is the energy obtained by single point calculation using M06-2X-SMD/BS2 on a structure optimized at the M06-2X-SMD/BS1 level; $\Delta G^{M06-2X-SMD/BS1}_{thermo}$ is a thermal correction to the free energy of the solute calculated at the M06-2X-SMD/BS1 level; and $\Delta G^{1\ atm \rightarrow 1M}$ stands for the free-energy change for compression of 1 mol of an ideal gas from 1 atm to the 1 M solution phase standard state. For selected stationery points of importance, we used an alternative methodology as outlined in eq. S2. In this case, we optimized structures with the larger basis set BS2 using the M06-2X-SMD method. $G^{M06-2X-SMD/BS2}$ is the Gibbs free energy calculated at the M06-2X-SMD/BS2 level. The energy profiles calculated based on these two alternatives are illustrated in Figs S5-S12.

$$G_{soln} = E^{M06-2X-SMD/BS2} + \Delta G^{M06-2X-SMD/BS1}_{thermo} + \Delta G^{1atm \rightarrow 1M}$$

$$G_{soln} = G^{M06-2X-SMD/BS2} + \Delta G^{1atm \rightarrow 1M}$$

We found that the relative Gibbs free energies obtained based on eqs S1 and S2 are nearly comparable with those obtained based on eq 1 (see the computational results given in manuscript). Indeed, the energetic trends are similar for all three methodologies. For example, each methodology allowed us to infer that the conventional mechanism (Figs 1 and S5) is unlikely to occur under the reaction conditions due to having a high overall activation barrier; the ligand exchange for formation of **7** through the stepwise mechanism is slightly more favorable than the concerted mechanism (Figs 3 and S6); both $\mathbf{TS_{10\text{-}11}}$ (Figs 4 and S7) and **TS** (Figs 5 and S8) are much lower in energy than $\mathbf{TS_{4\text{-}6}}$ (Figs 1 and S5), which indicates that our proposed mechanism is more favored over the conventional one.

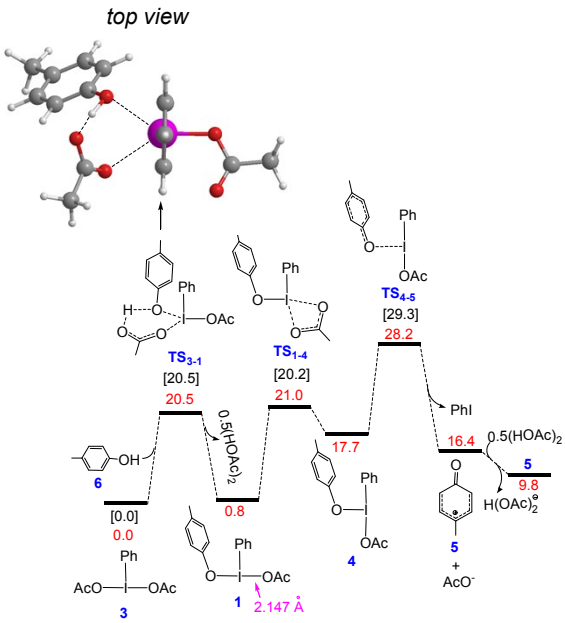

Fig. S5 A Gibbs free energy profile (kcal/mol) for oxidative dearomatization of a phenol by PIDA in MeCN through the conventional mechanism calculated based on the methodology represented by eq S1. The some values given in bracket are the relative Gibbs free energies calculated based on the methodology represented by eq S2.

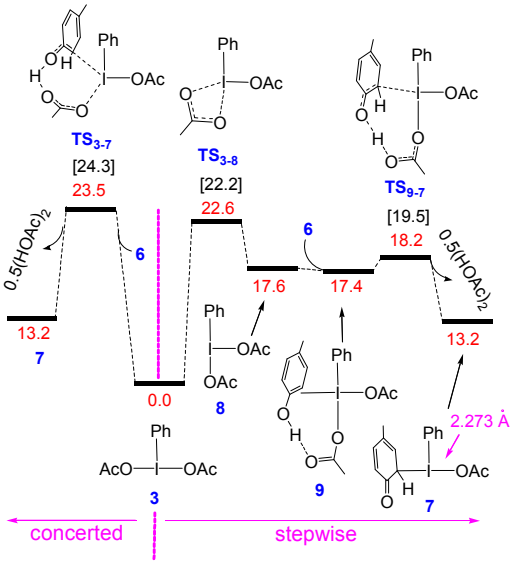

Fig. S6 Gibbs free energy profiles (kcal/mol) comparing two pathways concerted and stepwise for formation of **7** from **3** in MeCN calculated based on the methodology represented by eq S1. The some values given in bracket are the relative Gibbs free energies calculated based on the methodology represented by eq S2.

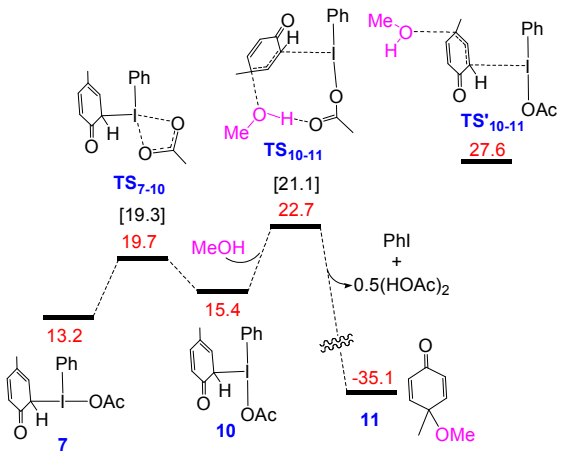

Fig. S7 Gibbs free energy profile (kcal/mol) for oxidative dearomatization of a phenol in MeCN starting from the key intermediate **7** via associative mechanism calculated based on the methodology represented by eq S1. The some values given in bracket are the relative Gibbs free energies calculated based on the methodology represented by eq S2.

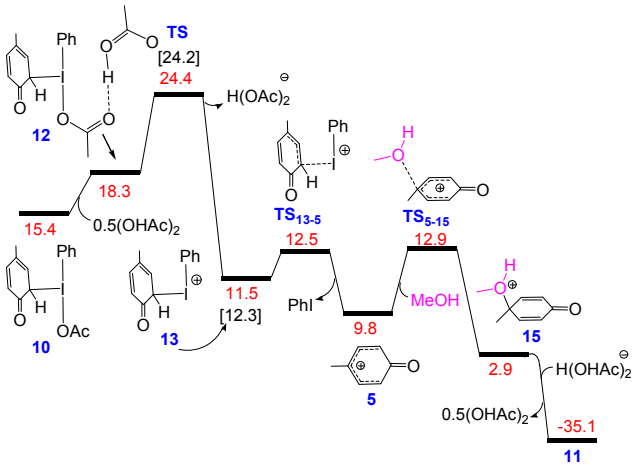

Fig. S8 Gibbs free energy profile (kcal/mol) for oxidative dearomatization of a phenol in MeCN starting from the key intermediate **10** via dissociative mechanism calculated based on the methodology represented by eq S1. The some values given in bracket are the relative Gibbs free energies calculated based on the methodology represented by eq S2.

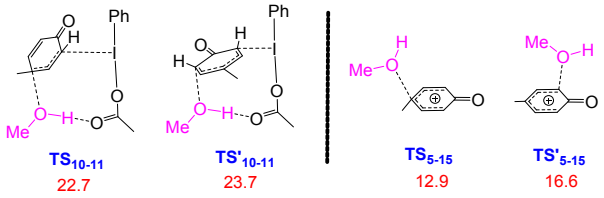

Fig. S9 Relative Gibbs free energy (kcal/mol) of transition structures relating to addition of MeOH to dearomatized phenol/phenoxenium calculated based on the methodology represented by eq S1.

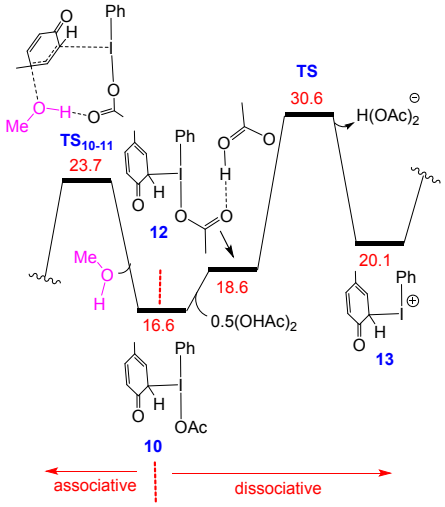

Fig. S10 Gibbs free energy profiles (kcal/mol) calculated based on the methodology represented by eq S1 comparing two pathways concerted and stepwise for phenol dearomatization in CH_2Cl_2.

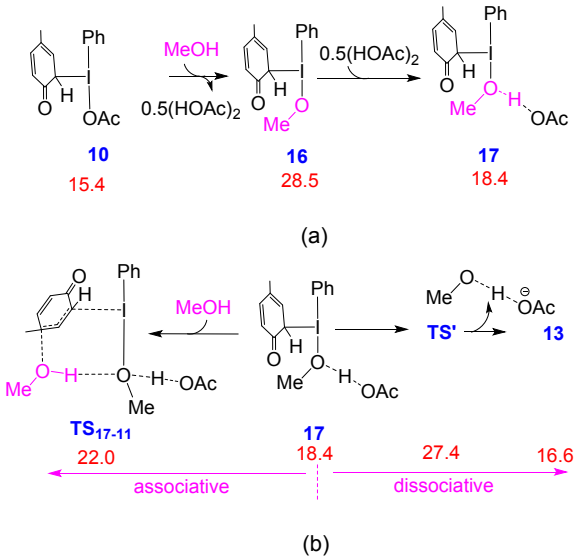

Fig. S11 (a) Relative Gibbs free energy (kcal/mol) of intermediates **10**, **16**, and **17** and (b) that of vital stationary points starting from **17** for two pathways concerted and stepwise in phenol dearomatization process calculated based on the methodology represented by eq S1 where MeCN was considered as the solvent.

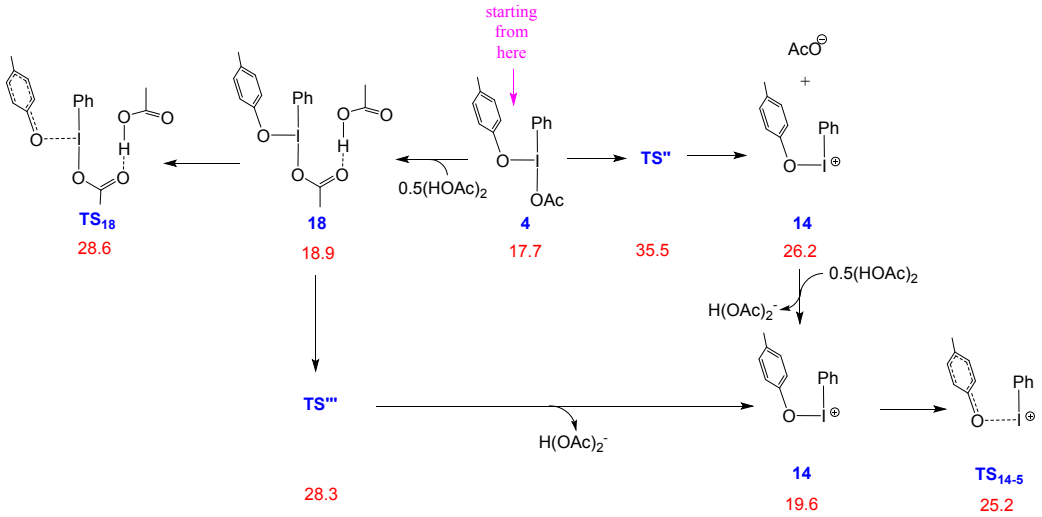

Fig. S12 Calculated mechanism of phenol dearomatization starting from **4** via different variants occurring through vital transition structures **TS_{18}**, **TS″** and **TS‴**. Free energies are calculated based on the methodology represented by eq S1.

Cartesian coordinates and total energies for the calculated structures in MeCN and CH_2Cl_2

2

E(M06-2X-SMD/BS1) = -817.6827651 au
H(M06-2X-SMD/BS1) = -817.38301 au
G(M06-2X-SMD/BS1) = -817.457269 au
E(M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -1104.297601 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -817.9771729 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -818.0667643 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1104.205093 au

I	-0.97005700	-0.65360600	-0.57329400
C	-0.45788000	1.31687000	-0.14454600
C	0.40084600	3.88023500	0.35451200
C	-0.61839400	2.27774800	-1.14016400
C	0.12179600	1.59612200	1.09073000
C	0.54919400	2.89980600	1.33412100
C	-0.17948300	3.57288300	-0.87598800
H	-1.06952400	2.02522100	-2.09380700
H	0.24235400	0.81910500	1.83826600
H	1.00504800	3.14264500	2.28830600
H	-0.29344900	4.33994700	-1.63494800
H	0.74120600	4.89209900	0.55000700
O	0.74284800	-0.93311200	-1.56050700
C	1.89409000	-0.89599900	-0.79940500
C	4.28416900	-0.82162100	0.65774900
C	2.27103500	-1.99920300	-0.03230100
C	2.68930900	0.24630200	-0.83546500
C	3.88117100	0.27155200	-0.11216800
C	3.45983600	-1.95511400	0.68523300
H	1.63274300	-2.87816700	-0.00932000
H	2.37158300	1.09859500	-1.42915100
H	4.50450600	1.16120100	-0.14454700
H	3.75715700	-2.81611900	1.27885800
C	5.56941600	-0.79586600	1.44360700
H	6.24950600	-1.58667100	1.10908800
H	5.38139500	-0.96039000	2.50998500
H	6.08185100	0.16306800	1.33152800
O	-2.92093800	0.03939900	0.64901500
C	-3.87143400	-0.72501500	0.81245000
O	-3.79246300	-1.93258500	0.28523200
C	-5.09814400	-0.34861400	1.57233300
H	-5.00706700	0.67119100	1.94113900
H	-5.22942700	-1.04250300	2.40855000
H	-5.96896100	-0.43574600	0.91490300
H	-4.59463900	-2.46244800	0.47159200

3

E(M06-2X-SMD/BS1) = -699.6057006 au
H(M06-2X-SMD/BS1) = -699.392574 au

G(M06-2X-SMD/BS1) = -699.457865 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -986.1839449 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -699.9089306 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -699.9291768 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -986.1603364 au

I	0.49530300	-0.73648400	-0.20466400
C	-0.63606100	1.03254600	-0.13977800
C	-2.16125400	3.32575000	-0.03941800
C	-0.39246300	1.95224500	0.87351200
C	-1.62055100	1.22241100	-1.10266900
C	-2.38780500	2.38521200	-1.04231500
C	-1.16701100	3.11028800	0.91367100
H	0.38140400	1.77534500	1.61215500
H	-1.79272600	0.48480900	-1.87928300
H	-3.15915400	2.55314500	-1.78710000
H	-0.99455300	3.83889300	1.69938100
H	-2.76197000	4.22883400	0.00064500
O	2.10159600	0.64949000	-0.01208100
C	3.25889400	0.02489400	0.04752100
O	3.35217900	-1.19272900	-0.01723000
C	4.43733400	0.95189000	0.19938900
H	4.32525200	1.53842200	1.11546500
H	4.46453500	1.64924700	-0.64242900
H	5.36187800	0.37590700	0.23636800
O	-1.32911000	-1.72782300	-0.51545400
C	-2.18808100	-1.75767400	0.49947600
O	-1.96964800	-1.25699500	1.58461800
C	-3.47087100	-2.46338100	0.13583900
H	-3.98760500	-1.88669500	-0.63763800
H	-3.25219200	-3.45190000	-0.27565700
H	-4.10886200	-2.55299100	1.01508600

6

E(M06-2X-SMD/BS1) = -346.635413 au
H(M06-2X-SMD/BS1) = -346.49362 au
G(M06-2X-SMD/BS1) = -346.533882 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -346.7802366 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -346.7754472 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -346.787896 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -346.7664619 au

O	-2.79768400	-0.09671700	0.00231200
C	-1.43916000	-0.01999000	0.00109000
C	1.37633400	0.01273500	-0.00332700
C	-0.72338500	-1.22042300	-0.00031500
C	-0.75331600	1.19341200	-0.00036600
C	0.64141000	1.19893300	-0.00283700
C	0.66543600	-1.19451200	-0.00282200
H	-1.26874000	-2.15920100	-0.00096100
H	-1.30843600	2.12847800	-0.00106900
H	1.16539200	2.15152600	-0.00504900

H	1.21288600	-2.13436500	-0.00517000
C	2.88395900	0.01866600	0.00367100
H	3.27374800	1.03480500	-0.10214400
H	3.28745300	-0.58684600	-0.81490100
H	3.27846200	-0.39681600	0.93785100
H	-3.16696200	0.80323900	0.00238700

TS_{3-1}

E(M06-2X-SMD/BS1) = -1046.224555 au
H(M06-2X-SMD/BS1) = -1045.870735 au
G(M06-2X-SMD/BS1) = -1045.956301 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1332.947434 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -1046.663025 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -1046.694066 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1332.910943 au

I	0.52116600	-0.94034200	-0.12595200
C	1.78946500	0.52782700	0.62159900
C	3.41363900	2.51923500	1.59592500
C	2.59374600	1.22798300	-0.27547800
C	1.76165300	0.80013500	1.98640200
C	2.59323000	1.80848700	2.47007400
C	3.41424200	2.23261300	0.23038600
H	2.57287900	0.99884800	-1.33479900
H	1.10352600	0.25027000	2.65019400
H	2.59110600	2.03968600	3.53018400
H	4.05140700	2.79275500	-0.44636700
H	4.05421500	3.30683500	1.98003600
O	-1.22247500	0.67300600	0.99816700
C	-2.48193800	0.27006400	0.70378100
C	-5.08652700	-0.65293700	0.11815400
C	-3.34373100	1.03810600	-0.09251600
C	-2.92909500	-0.95708300	1.20312200
C	-4.21481100	-1.40610000	0.90746200
C	-4.62463000	0.57546300	-0.37093200
H	-3.00205900	1.99441100	-0.47673500
H	-2.26393700	-1.54423800	1.82991500
H	-4.54750000	-2.36231900	1.30452000
H	-5.28420800	1.18400900	-0.98614500
C	-6.48136200	-1.13229000	-0.19489700
H	-6.65817600	-2.12754200	0.22242600
H	-6.65159800	-1.18341100	-1.27586700
H	-7.23704600	-0.45503200	0.21870500
O	-0.23612900	1.15410500	-1.62699100
C	-0.26251700	2.35678400	-1.27720800
O	-0.61580500	2.76740600	-0.12481700
C	0.19433000	3.41408200	-2.26302500
H	0.15713000	3.03537000	-3.28545100
H	1.23129000	3.67917300	-2.02487900
H	-0.41196500	4.31757400	-2.16788000
O	1.87606500	-2.40752600	0.13003600

C	2.92360600	-2.43873500	-0.72872000
O	3.09531400	-1.61454400	-1.59164500
C	3.81177300	-3.61520500	-0.43712900
H	4.18398600	-3.54538800	0.58837600
H	3.23574600	-4.53997100	-0.52518500
H	4.64477000	-3.62112500	-1.13936100
H	-0.99354600	1.62805600	0.55375400

1

E(M06-2X-SMD/BS1) = -817.2493729 au
H(M06-2X-SMD/BS1) = -816.962376 au
G(M06-2X-SMD/BS1) = -817.035724 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1103.863034 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -817.6037906 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -817.6264878 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1103.836382 au

I	-1.04535100	-0.61845400	-0.53372800
C	-0.58125600	1.39204600	-0.10989000
C	0.09663000	4.00895000	0.42406600
C	0.02650100	2.14230600	-1.10914100
C	-0.85716200	1.90868800	1.15059500
C	-0.51207400	3.23394600	1.40926200
C	0.36539300	3.46515600	-0.83002700
H	0.23899200	1.70424100	-2.07844300
H	-1.33786000	1.30080400	1.90811700
H	-0.71562800	3.65556900	2.38813000
H	0.83648600	4.06784800	-1.59958600
H	0.36263500	5.03947800	0.63540400
O	0.76403000	-0.73953300	-1.50335300
C	1.90346100	-0.78615900	-0.75334000
C	4.31607800	-0.87870300	0.70385100
C	2.14743200	-1.82793200	0.14449900
C	2.86840300	0.21328700	-0.91738800
C	4.05780900	0.15752300	-0.19959200
C	3.34007200	-1.86517700	0.86228400
H	1.40454200	-2.61092100	0.27007100
H	2.67509100	1.02045100	-1.61675500
H	4.80135600	0.93837500	-0.34128100
H	3.51626200	-2.68295600	1.55659200
C	5.61758200	-0.93198700	1.46394800
H	6.45287900	-1.18200000	0.80058500
H	5.58257300	-1.68633600	2.25432300
H	5.84726000	0.03384900	1.92473300
O	-2.85645400	-0.08020600	0.47750900
C	-3.65371400	-1.12000400	0.58474500
O	-3.36771700	-2.22029500	0.13194600
C	-4.94062400	-0.82458800	1.31653900
H	-5.46377800	-0.00249900	0.82243500
H	-4.71340800	-0.50806900	2.33785700
H	-5.56984300	-1.71360800	1.33412200

TS_{1-4}

E(M06-2X-SMD/BS1) = -817.2156913 au
H(M06-2X-SMD/BS1) = -816.931024 au
G(M06-2X-SMD/BS1) = -817.001312 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1103.831668 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -817.5747988 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -817.6008965 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1103.800139 au

I	-1.22854500	0.27197200	-0.16285400
C	0.11421400	1.86203500	0.15459300
C	1.98721500	3.87238900	0.50981800
C	0.11967900	2.95551600	-0.71588000
C	1.03241700	1.76680700	1.20364600
C	1.97303200	2.78054200	1.37665900
C	1.06415500	3.96185400	-0.53339500
H	-0.60093900	3.01559600	-1.52614500
H	1.01610200	0.90929200	1.87053800
H	2.69356800	2.71584500	2.18584600
H	1.08013000	4.81520900	-1.20405500
H	2.72150000	4.66016900	0.64741200
O	0.06410000	-0.60399900	-1.42746800
C	1.20234500	-1.11978400	-0.85299600
C	3.56039300	-2.19880400	0.20541800
C	1.15343500	-2.30977600	-0.12381100
C	2.41180500	-0.45481100	-1.04052300
C	3.58198200	-1.00463400	-0.51805800
C	2.32735700	-2.83917100	0.39600300
H	0.19592400	-2.80171800	0.02560800
H	2.42491400	0.47779100	-1.59679400
H	4.52679500	-0.48965300	-0.67075200
H	2.29086600	-3.76719100	0.96125000
C	4.82427200	-2.79680000	0.76659200
H	5.67006900	-2.11431700	0.64917900
H	5.07352200	-3.73447100	0.25727100
H	4.71293600	-3.02635400	1.83130300
O	-2.85898500	-1.62235600	-0.43348300
C	-3.71476800	-1.10362000	0.34358400
O	-3.55351500	0.01660300	0.90247600
C	-4.98066500	-1.88905200	0.62563300
H	-4.73101000	-2.75266400	1.25087500
H	-5.39924500	-2.26772900	-0.31043600
H	-5.71628300	-1.27245800	1.14427100

4

E(M06-2X-SMD/BS1) = -817.2220633 au
H(M06-2X-SMD/BS1) = -816.935238 au
G(M06-2X-SMD/BS1) = -817.009227 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1103.835385 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -817.5755771 au

E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -817.601307 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1103.804902 au

I	-1.13811600	0.79976600	0.06136500
C	0.66187700	1.91408600	0.17014300
C	3.06542600	3.30207100	0.29988300
C	0.97673500	2.84375400	-0.82430600
C	1.54297100	1.67352700	1.22644400
C	2.74707400	2.37470900	1.28995300
C	2.18269000	3.53713100	-0.75578500
H	0.28815700	3.02257200	-1.64540800
H	1.29465700	0.94243500	1.99089000
H	3.43617900	2.19139500	2.10855300
H	2.43370100	4.26123700	-1.52477600
H	4.00428200	3.84510300	0.34926000
O	-0.18206000	-0.31534600	-1.28116400
C	0.73722900	-1.20785400	-0.77457600
C	2.63624300	-3.06032400	0.11669200
C	0.31664900	-2.36247000	-0.11064400
C	2.09108100	-0.96203000	-0.98422700
C	3.02994200	-1.89564700	-0.54441200
C	1.26596000	-3.27584700	0.32739900
H	-0.74683900	-2.51987500	0.04707900
H	2.39376000	-0.05199000	-1.49368900
H	4.08704900	-1.70817600	-0.71345500
H	0.94274400	-4.17769000	0.84177000
C	3.64715800	-4.07090600	0.59286500
H	3.52791600	-5.02338200	0.06465600
H	3.52512500	-4.27635500	1.66153000
H	4.66806700	-3.71725300	0.42682800
O	-2.60691100	-0.88405000	-0.48575700
C	-3.69267000	-0.68695500	0.19126400
O	-3.86876800	0.28757600	0.92900300
C	-4.75225200	-1.75648500	0.01806800
H	-4.35795900	-2.71944200	0.35648100
H	-5.00517900	-1.85797600	-1.04119200
H	-5.64625200	-1.50422500	0.58989900

TS_{4-5}

E(M06-2X-SMD/BS1) = -817.1984822 au
H(M06-2X-SMD/BS1) = -816.913602 au
G(M06-2X-SMD/BS1) = -816.986111 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1103.818077 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -817.5547694 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -817.5955687 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1103.766445 au

I	1.47246600	0.40837600	-0.06406800
C	-0.44863700	1.20798300	-0.15836600
C	-3.06209300	2.19229700	-0.25862300
C	-0.96439800	1.97040600	0.91313300
C	-1.25770400	0.95293300	-1.27865100

C	-2.56087700	1.43826700	-1.32080600
C	-2.25384200	2.47718200	0.84781000
H	-0.34234400	2.16397100	1.78227400
H	-0.85871700	0.38424700	-2.11391400
H	-3.18733100	1.22820400	-2.18294300
H	-2.64334000	3.07242500	1.66776400
H	-4.07886600	2.57190300	-0.29773400
O	0.08308900	-1.84496200	0.58313900
C	-1.13239500	-1.61891600	0.41180900
C	-3.89841900	-1.16851500	0.07650200
C	-1.82570200	-2.07087200	-0.78995700
C	-1.90516200	-0.90227500	1.41375500
C	-3.24917800	-0.70449700	1.24260000
C	-3.16844900	-1.88458600	-0.91802600
H	-1.23673700	-2.57809700	-1.54827000
H	-1.38041400	-0.56434100	2.30203300
H	-3.82951600	-0.16906500	1.98743100
H	-3.69857300	-2.23757300	-1.79755100
C	-5.35505400	-0.93283900	-0.12354100
H	-5.89095100	-1.88569500	-0.01464200
H	-5.54874900	-0.57873600	-1.14164400
H	-5.75572900	-0.22099700	0.59991500
O	4.53381000	0.85238700	-0.38780300
C	4.56185400	-0.34421200	-0.04802300
O	3.54866900	-1.06577300	0.21961100
C	5.91407500	-1.05223500	0.07423300
H	6.73640500	-0.38174200	-0.18364200
H	5.93618200	-1.92651300	-0.58423500
H	6.04929300	-1.41584900	1.09806800

Acetate
E(M06-2X-SMD/BS1) = -228.4937093 au
H(M06-2X-SMD/BS1) = -228.43999 au
G(M06-2X-SMD/BS1) = -228.470334 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -228.6167882 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -228.4926757 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -228.5873396 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -228.5207184 au

O	-0.70269300	1.15159400	0.00154000
C	-0.20455100	0.00069400	-0.00744400
O	-0.80177200	-1.10080000	0.00169200
C	1.34451600	-0.04752100	-0.00239400
H	1.71754300	0.28121100	0.97568900
H	1.75176800	0.64695400	-0.74525200
H	1.72660900	-1.05355900	-0.19726300

PhI
E(M06-2X-SMD/BS1) = -242.8837998 au
H(M06-2X-SMD/BS1) = -242.785911au
G(M06-2X-SMD/BS1) = -242.824367 au

E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -529.2646575 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -243.0273603 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -243.0351596 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -529.2565366 au

I	-1.54906800	0.00000100	-0.00002000
C	0.55886400	0.00011200	0.00002300
C	3.33568000	-0.00016000	-0.00016800
C	1.24281600	-1.21414900	0.00010700
C	1.24307800	1.21432800	0.00011000
C	2.63736400	1.20584100	0.00001800
C	2.63724600	-1.20593500	0.00001800
H	0.69960700	-2.15304100	0.00027800
H	0.69974000	2.15315900	0.00030200
H	3.17518400	2.14899300	0.00005600
H	3.17464600	-2.14932700	0.00008900
H	4.42112300	-0.00004100	-0.00031900

5

E(M06-2X-SMD/BS1) = -345.7865336 au
H(M06-2X-SMD/BS1) = -345.657469 au
G(M06-2X-SMD/BS1) = -345.697723 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -345.9208252 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -345.8497675 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -345.950055 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -345.818740 au

O	2.74254600	-0.00221100	0.01114500
C	1.52985400	-0.00118100	0.00305100
C	-1.28653600	0.00290100	-0.02393300
C	0.76122700	-1.27837700	-0.00080500
C	0.76421900	1.27816500	-0.00091900
C	-0.58360800	1.25981600	-0.01394000
C	-0.58620800	-1.25620400	-0.01452300
H	1.33638100	-2.19888900	0.00530800
H	1.34190000	2.19712300	0.00436400
H	-1.16868800	2.17303100	-0.01997200
H	-1.17376000	-2.16794300	-0.02079800
C	-2.75032000	0.00084400	0.00452000
H	-3.01920600	-0.05647600	1.07754500
H	-3.17036600	-0.88965900	-0.46875100
H	-3.17839400	0.92472000	-0.38756300

7

E(M06-2X-SMD/BS1) = -817.2248236 au
H(M06-2X-SMD/BS1) = -816.938002 au
G(M06-2X-SMD/BS1) = -817.012432 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1103.842113 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -817.5773074 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -817.6079162 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1103.806649 au

I	0.47107600	0.61655700	-0.27383000

C	0.61152400	-1.47477100	-0.27076200
C	0.71784400	-4.23165100	-0.26403300
C	0.69900400	-2.14578900	-1.48624900
C	0.57692300	-2.14480200	0.94890000
C	0.63418100	-3.53726700	0.94233000
C	0.75023100	-3.53957000	-1.47303800
H	0.72412500	-1.59887400	-2.42325500
H	0.50334600	-1.59646100	1.88208200
H	0.60791900	-4.07715100	1.88349400
H	0.81841100	-4.07980700	-2.41189300
H	0.75775600	-5.31632600	-0.26130500
O	-1.76260700	2.69523300	-1.69147700
C	-2.13697000	1.84047200	-0.89190300
C	-3.18761600	-0.23412300	0.84427300
C	-2.96226400	2.15972100	0.27670700
C	-1.69455800	0.41419100	-1.00989200
C	-2.37673400	-0.58519400	-0.17723900
C	-3.44529300	1.18178300	1.07432100
H	-3.20088000	3.20580500	0.44295800
H	-1.53019500	0.11918600	-2.04749700
H	-2.17945300	-1.63454500	-0.38383600
H	-4.07643200	1.44520700	1.92123600
C	-3.84749700	-1.23736400	1.74742000
H	-4.93859600	-1.14087100	1.71209400
H	-3.54509700	-1.07978100	2.78931200
H	-3.58067500	-2.25847800	1.46267700
O	2.61343800	0.33623200	0.43326200
C	3.15381600	1.49530900	0.65284100
O	2.57374800	2.56724500	0.47908800
C	4.58545300	1.42985800	1.14871400
H	5.20710400	0.92123500	0.40612200
H	4.62889600	0.84496300	2.07185500
H	4.97186000	2.43391300	1.32765200

$TS_{1\text{-}7}$

E(M06-2X-SMD/BS1) = -817.2057459 au
H(M06-2X-SMD/BS1) = -816.920673 au
G(M06-2X-SMD/BS1) = -816.991545 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1103.824538 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -817.5596596 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -817.5864485 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1103.793000 au

I	0.68945700	-0.98375000	-0.23904000
C	0.15857100	1.02804600	-0.20808900
C	-0.67407900	3.65766400	-0.14083800
C	-0.29275300	1.62174500	-1.38501100
C	0.17814200	1.70898900	1.00836500
C	-0.23545700	3.03883400	1.03053000
C	-0.70364700	2.95316400	-1.34353600
H	-0.32504700	1.05899500	-2.31254300

H	0.52097600	1.21417100	1.91031900
H	-0.21836100	3.58869700	1.96610300
H	-1.05132500	3.43422200	-2.25211500
H	-0.99977000	4.69281500	-0.11402700
O	-1.20477100	-3.48405700	0.15414100
C	-1.65158100	-2.32117700	0.17194300
C	-2.97721500	0.25735700	0.26755800
C	-2.08568800	-1.60404300	-1.02693700
C	-1.69624000	-1.49181100	1.37753300
C	-2.40058700	-0.29878000	1.41925900
C	-2.78452500	-0.40999800	-0.95153000
H	-1.96308100	-2.11651400	-1.97783100
H	-1.27410800	-1.91955700	2.28343900
H	-2.47581900	0.24093800	2.36091300
H	-3.16163500	0.04314400	-1.86561400
C	-3.73086900	1.55650300	0.33563600
H	-4.72541900	1.41178900	0.77509200
H	-3.86505600	1.98972500	-0.65949000
H	-3.20371300	2.28425800	0.96199000
O	2.68787400	-0.33437200	-0.69272200
C	3.37417500	0.15856900	0.32638200
O	2.93713400	0.28131800	1.45565400
C	4.77325900	0.56524200	-0.07809900
H	5.29287700	-0.28803500	-0.52149800
H	5.31955300	0.92619800	0.79353700
H	4.71779200	1.35297500	-0.83474800

8

E(M06-2X-SMD/BS1) = -699.5752695 au
H(M06-2X-SMD/BS1) = -699.362294 au
G(M06-2X-SMD/BS1) = -699.429565 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -986.1537374 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -699.8784708 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -699.9012784 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -986.126358 au

I	-0.32268400	-0.60896500	-0.01427100
C	1.79736200	-0.49794200	0.01860300
C	4.57168700	-0.40108500	0.11092200
C	2.43067100	0.12019700	1.09956700
C	2.54186500	-1.07022100	-1.01404500
C	3.93421200	-1.02133600	-0.96262500
C	3.82246300	0.16974600	1.13984900
H	1.84309000	0.56167400	1.89965500
H	2.04165800	-1.54939100	-1.85064800
H	4.51919700	-1.46550400	-1.76209900
H	4.32119200	0.65032100	1.97587500
H	5.65614800	-0.36341700	0.14707200
O	-2.88588500	-1.89566700	0.50747600
C	-3.25893300	-0.79457800	0.09758700
O	-2.44391800	0.13131800	-0.30475800

C	-4.72334000	-0.41689300	0.02534200
H	-4.90522600	0.46471600	0.64688200
H	-5.34612500	-1.24454100	0.36695300
H	-4.98533800	-0.15521500	-1.00386400
O	-0.20558500	1.20501000	-0.84031900
C	-0.33189100	2.24895300	0.00972100
O	-0.41548400	2.12646600	1.20589800
C	-0.34602500	3.54383000	-0.75352300
H	0.52990700	3.60340200	-1.40386400
H	-1.23927100	3.57577600	-1.38361500
H	-0.35443100	4.37628300	-0.05075400

TS_{3-8}

E(M06-2X-SMD/BS1) = -699.5672106 au
H(M06-2X-SMD/BS1) = -699.35557 au
G(M06-2X-SMD/BS1) = -699.419876 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -986.1474918 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -699.8770033 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -699.8991244 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -986.1201562 au

I	-0.49513800	-0.20785600	-0.11828300
C	1.55636500	-0.69468500	-0.02535500
C	4.23337000	-1.39118200	0.10265900
C	2.24694900	-0.53855300	1.17910000
C	2.18603000	-1.20582600	-1.16242100
C	3.53412100	-1.54987500	-1.09356800
C	3.59357400	-0.88836700	1.23602700
H	1.74152900	-0.13989800	2.05282800
H	1.63212400	-1.33125600	-2.08796200
H	4.03578100	-1.94453100	-1.97143500
H	4.14281100	-0.76877900	2.16457600
H	5.28318600	-1.66328000	0.15324500
O	-2.44188500	-1.78412300	0.38044200
C	-3.27533200	-0.86863100	0.13333300
O	-2.93456400	0.30262400	-0.21307800
C	-4.75614000	-1.16777300	0.24452600
H	-5.22518700	-1.03342500	-0.73501200
H	-5.22110400	-0.45662000	0.93334800
H	-4.92415500	-2.18716400	0.59457300
O	-0.09361600	1.65342600	-0.77242700
C	0.38473900	2.53134300	0.14119200
O	0.61376100	2.23525100	1.28696500
C	0.58536100	3.88383600	-0.48286300
H	1.28773500	3.80047800	-1.31643600
H	-0.36635000	4.24911800	-0.87728800
H	0.97216200	4.57255200	0.26756100

9

E(M06-2X-SMD/BS1) = -1046.234201 au
H(M06-2X-SMD/BS1) = -1045.877611 au

G(M06-2X-SMD/BS1) = -1045.964432 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1332.953787 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -1046.673317 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -1046.698994 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1332.923317 au

I	0.77395200	0.16866000	-0.41306000
C	-1.03696700	1.23083300	-0.21418200
C	-3.49139700	2.48349400	0.08715500
C	-1.75860300	1.60664000	-1.34932900
C	-1.53035300	1.47090400	1.06906500
C	-2.76553000	2.10235600	1.21438800
C	-2.99001000	2.23785100	-1.19241400
H	-1.36673600	1.40262500	-2.34155900
H	-0.96049900	1.16688500	1.94232800
H	-3.15926700	2.29259000	2.20800600
H	-3.56002000	2.53291200	-2.06798700
H	-4.45399200	2.97188900	0.20459700
O	0.37207500	-2.88273100	1.45747200
C	-0.77512700	-2.46602500	0.88289800
C	-3.21603700	-1.56103700	-0.22773800
C	-0.93260300	-2.36829700	-0.50913700
C	-1.84633400	-2.11466700	1.71469600
C	-3.04004600	-1.67333500	1.16045900
C	-2.14523400	-1.91666900	-1.04371800
H	-0.12347500	-2.68461700	-1.16276400
H	-1.71804400	-2.18439400	2.79049900
H	-3.85782700	-1.39409900	1.82133900
H	-2.24549700	-1.84017400	-2.12404300
C	-4.52191300	-1.07761300	-0.80426400
H	-5.27155100	-1.87783400	-0.81489300
H	-4.39340900	-0.72905300	-1.83317500
H	-4.93317500	-0.25381700	-0.21222900
O	1.70995400	1.93117100	-0.50511900
C	2.07528800	2.46927500	0.68183700
O	1.79966500	1.97476400	1.74588500
C	2.84662000	3.74071500	0.46525400
H	3.76837700	3.51352100	-0.07724300
H	3.08015200	4.18927000	1.43023900
H	2.25755200	4.43236100	-0.14200600
H	1.10048800	-2.85510500	0.79313600
O	2.24108300	-2.37936600	-0.41912400
C	3.21370100	-1.58809300	-0.40041000
O	3.09345700	-0.32185100	-0.46941700
C	4.61729500	-2.13707700	-0.26319000
H	4.81998100	-2.30271000	0.80067100
H	4.69632000	-3.09717800	-0.77680800
H	5.35481300	-1.43346400	-0.65173000

$TS_{9\text{-}7}$
E(M06-2X-SMD/BS1) = -1046.227914 au

H(M06-2X-SMD/BS1) = -1045.874759 au
G(M06-2X-SMD/BS1) = -1045.960545 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1332.950148 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -1046.665580 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -1046.696990 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1332.913760 au

I	0.53072000	0.48925900	-0.29205700
C	-1.54159400	0.72209700	-0.30175500
C	-4.29156700	0.97569300	-0.30779600
C	-2.21422400	0.77408800	-1.52364700
C	-2.21631000	0.78700400	0.91645300
C	-3.60495300	0.91452900	0.90368700
C	-3.60003100	0.90592800	-1.51838800
H	-1.66644300	0.71001900	-2.45851500
H	-1.66946600	0.74641900	1.85212300
H	-4.14645100	0.96835700	1.84268300
H	-4.13863900	0.95065700	-2.45950200
H	-5.37250200	1.07647800	-0.31024900
O	1.60728900	-2.07859000	1.65785500
C	0.45122300	-2.20957400	1.06123800
C	-2.09437500	-2.55222000	-0.19243700
C	0.30554300	-2.13667700	-0.35757000
C	-0.72369700	-2.37817100	1.83647700
C	-1.94286000	-2.54396000	1.21986900
C	-0.96317700	-2.36875200	-0.95381400
H	1.20424000	-2.18820300	-0.96935100
H	-0.62975600	-2.39249500	2.91754300
H	-2.82993400	-2.67573500	1.83638200
H	-1.03078100	-2.36375900	-2.03907800
C	-3.45743900	-2.73622700	-0.80243100
H	-3.86416200	-3.72777100	-0.57326900
H	-3.41997600	-2.62578000	-1.88965500
H	-4.16322900	-1.99687100	-0.40729800
O	0.80308000	2.53333300	-0.44094900
C	0.55677900	3.24932800	0.66553500
O	0.15219200	2.76878700	1.70027100
C	0.84267800	4.71178300	0.44371700
H	1.89136800	4.84007200	0.16294900
H	0.62726500	5.26762400	1.35598800
H	0.22605100	5.08451000	-0.37847400
H	2.43134900	-2.00696200	0.94952000
O	3.49307600	-2.01735000	0.09537200
C	3.86586500	-0.88643500	-0.36761700
O	3.21842600	0.17669700	-0.30101400
C	5.22153700	-0.88628800	-1.05292200
H	5.98726800	-1.22505300	-0.34867500
H	5.20804800	-1.59618900	-1.88565500
H	5.47472100	0.10806500	-1.42233500

$(HOAc)_2$

E(M06-2X-SMD/BS1) = -458.0022901 au
H(M06-2X-SMD/BS1) = -457.864074 au
G(M06-2X-SMD/BS1) = -457.912184 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -458.2153001 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -458.187081 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -458.195926 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -458.204600 au

O	1.24317900	1.06781200	0.00003800
C	1.93452600	0.05578000	-0.00002200
O	1.43022900	-1.16207400	0.00010600
C	3.43174900	0.08189400	-0.00013400
H	3.78729300	1.11114100	-0.00115600
H	3.80320600	-0.44596700	-0.88289700
H	3.80319100	-0.44411000	0.88375800
H	0.43221100	-1.11104900	0.00028000
O	-1.24319200	-1.06782000	-0.00010400
C	-1.93452900	-0.05578100	-0.00005800
O	-1.43022200	1.16206800	0.00022000
C	-3.43174400	-0.08187300	-0.00015600
H	-3.78728900	-1.11111800	-0.00190700
H	-3.80325600	0.44667000	-0.88248300
H	-3.80312000	0.44345400	0.88417200
H	-0.43220300	1.11097900	0.00036400

$TS_{7\text{-}10}$
E(M06-2X-SMD/BS1) = -817.2124329 au
H(M06-2X-SMD/BS1) = -816.926801 au
G(M06-2X-SMD/BS1) = -816.998902 au
E(M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -1103.832767 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -817.567315 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -817.599554 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1103.793280 au

I	0.05019900	0.59760600	-0.16232100
C	-2.04381600	0.43740100	-0.04468100
C	-4.79903500	0.27441100	0.12070700
C	-2.63104200	0.07330200	1.16681900
C	-2.81006500	0.72727200	-1.17375000
C	-4.19692600	0.63724200	-1.08436900
C	-4.02043800	-0.00464400	1.24250400
H	-2.01675300	-0.14830400	2.03399000
H	-2.33313600	1.01516100	-2.10547300
H	-4.80607300	0.85482100	-1.95601000
H	-4.49180200	-0.28558600	2.17901000
H	-5.88078700	0.21067200	0.18529200
O	-1.56504200	-2.59732900	0.09761500
C	-0.36613500	-2.36537800	0.11667600
C	2.49774300	-2.28735700	-0.22351200
C	0.53397100	-2.86876100	1.16187500
C	0.27854000	-1.50953000	-0.94482300
C	1.73137000	-1.66725700	-1.14385400

C	1.86888000	-2.84297500	0.97578200
H	0.07897200	-3.33143500	2.03194000
H	-0.31975500	-1.46107300	-1.85479100
H	2.17166600	-1.22468400	-2.03303500
H	2.52632900	-3.27282600	1.72855100
C	3.98422000	-2.43118400	-0.36740900
H	4.27796000	-3.48612400	-0.33047200
H	4.49688300	-1.92470100	0.45862100
H	4.33482600	-2.00235200	-1.30898000
O	2.56407600	1.54859400	-0.11320500
C	2.19134200	2.68229600	0.28942100
O	0.99390400	3.00912800	0.52390600
C	3.25498000	3.75040100	0.52808100
H	3.28271100	4.00231100	1.59329700
H	2.99231100	4.66260700	-0.01585000
H	4.24104300	3.40382300	0.21358600

TS_{13-5}

E(M06-2X-SMD/BS1) = -588.6891223 au
H(M06-2X-SMD/BS1) = -588.461113 au
G(M06-2X-SMD/BS1) = -588.517309 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -875.2004948 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -588.895905 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -588.988414 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -875.106895 au

I	0.95292900	-1.52075600	-0.02474000
C	-1.02744800	-0.90967500	0.10408500
C	-3.68093300	-0.13615000	0.27951300
C	-1.80388100	-0.86400400	-1.05841700
C	-1.55408200	-0.55511100	1.35021500
C	-2.89044100	-0.17355700	1.42959000
C	-3.13713200	-0.47495800	-0.95999200
H	-1.37670800	-1.14027200	-2.01680400
H	-0.93278500	-0.58646500	2.23915300
H	-3.31268800	0.09476700	2.39265900
H	-3.75045600	-0.44073100	-1.85462600
H	-4.72280000	0.16003900	0.34972600
O	3.50790500	1.26344500	0.29213900
C	2.30154000	1.33874900	0.16988000
C	-0.37465500	2.11077900	-0.37245500
C	1.41263600	1.79372500	1.26336800
C	1.63501300	1.03659300	-1.13901200
C	0.38058500	1.54424700	-1.40647700
C	0.15077400	2.17327800	0.98176500
H	1.84195700	1.87742900	2.25658200
H	2.27037700	0.63807000	-1.92454500
H	-0.04973200	1.46397700	-2.39924900
H	-0.50352200	2.56239800	1.75671100
C	-1.71827500	2.67708900	-0.62027000
H	-1.71583800	3.74076400	-0.34615900

H	-2.44557200	2.19379500	0.04784500
H	-2.03292200	2.56269000	-1.65792500

MeOH
E(M06-2X-SMD/BS1) = -115.6586704 au
H(M06-2X-SMD/BS1) = -115.602542 au
G(M06-2X-SMD/BS1) = -115.629469 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -115.720563 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -115.7121552 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -115.7169973 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -115.7150216 au

O	-0.74685300	0.12384000	0.00000000
H	-1.12829200	-0.76739800	0.00000000
C	0.66066400	-0.01927900	0.00000000
H	1.08753600	0.98681500	-0.00000100
H	1.02579800	-0.54723100	0.89089100
H	1.02579800	-0.54723200	-0.89089000

10
E(M06-2X-SMD/BS1) = -817.2219833 au
H(M06-2X-SMD/BS1) = -816.935093 au
G(M06-2X-SMD/BS1) = -817.009797 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1103.838394 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -817.5726523 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -817.6032471 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1103.80293 au

I	0.39841700	-0.82736900	-0.16211700
C	2.42003500	-0.14288600	-0.10602100
C	5.07670600	0.66932200	-0.01826400
C	2.99996100	0.19104000	1.11925100
C	3.15917600	-0.07606800	-1.28602900
C	4.49349200	0.32939000	-1.23731400
C	4.33026700	0.60364600	1.15866900
H	2.41298900	0.13663700	2.03285200
H	2.70153900	-0.33556900	-2.23648000
H	5.07360900	0.38287600	-2.15356400
H	4.78506400	0.86775600	2.10858400
H	6.11429000	0.98690600	0.01604000
O	-0.75335600	0.49870200	2.61282800
C	-1.19246300	1.03036800	1.60930600
C	-2.17534000	2.32476100	-0.80090500
C	-2.53147600	1.62760100	1.54625000
C	-0.32475600	1.16311500	0.35559200
C	-0.93353100	1.81355100	-0.83063200
C	-2.97558000	2.21923800	0.42409600
H	-3.13957500	1.55123600	2.44217600
H	0.61659000	1.64708700	0.63731500
H	-0.31289300	1.90420200	-1.71857500
H	-3.97610700	2.64631300	0.40096600
C	-2.79291300	3.02850300	-1.97459800

H	-3.06648500	4.05610900	-1.70965800
H	-3.71382600	2.52041500	-2.28337000
H	-2.10911300	3.05752200	-2.82618700
O	-1.95527300	-0.98839400	-0.05185900
C	-2.33306500	-2.20635300	-0.23791700
O	-1.56847000	-3.14244400	-0.49305000
C	-3.83280200	-2.42774600	-0.12070900
H	-4.35440500	-1.80413300	-0.85314300
H	-4.17247000	-2.11811200	0.87240400
H	-4.08477900	-3.47649900	-0.28513400

$TS_{10\text{-}11}$

E(M06-2X-SMD/BS1) = -932.8873748 au
H(M06-2X-SMD/BS1) = -932.543978 au
G(M06-2X-SMD/BS1) = -932.625632 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1219.564613 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -933.2968493 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -933.3283468 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1219.527611 au

I	-0.43193200	-1.27925200	0.33614900
C	-2.40139200	-0.52624500	0.31544600
C	-4.95729700	0.56922300	0.26682900
C	-3.45832800	-1.26617600	-0.21643400
C	-2.61097400	0.75952800	0.82086700
C	-3.89508400	1.30349400	0.79241900
C	-4.73801800	-0.71318500	-0.23541900
H	-3.28676000	-2.26304100	-0.61101500
H	-1.77388000	1.32376300	1.22660600
H	-4.06350600	2.30229100	1.18407100
H	-5.56362800	-1.28679200	-0.64591500
H	-5.95569400	0.99526200	0.24851500
O	1.36354000	-1.24250400	-2.95991300
C	1.22563400	-0.28225800	-2.22992900
C	0.88164500	2.29145700	-1.08881900
C	2.36754100	0.42412000	-1.60719800
C	-0.13429500	0.30638900	-1.98322800
C	-0.25353200	1.60624700	-1.54420400
C	2.18661100	1.64439200	-1.07450700
H	3.33477000	-0.06468900	-1.64962000
H	-0.97060300	-0.22202600	-2.43262200
H	-1.22083400	2.09661700	-1.51698300
H	3.01447400	2.19642400	-0.63968400
C	0.79907400	3.73310900	-0.75402800
H	0.95610300	4.29756500	-1.68551700
H	1.58259700	4.03205200	-0.05543400
H	-0.18741700	3.99669100	-0.36618100
O	2.16385800	-1.88331500	0.23039400
C	2.89507500	-1.18654600	0.98524100
O	2.55130400	-0.16980700	1.64019500
C	4.36628200	-1.59086700	1.08485800

H	4.95697600	-0.93072000	0.43843000
H	4.51894700	-2.62171500	0.75971000
H	4.73082900	-1.46041600	2.10709000
H	1.27879100	0.90099900	1.40414300
O	0.73172300	1.73416700	1.40410300
C	1.43028800	2.64352100	2.22495300
H	2.43429500	2.86986100	1.83719100
H	0.86018600	3.57591700	2.27485800
H	1.54395200	2.25677300	3.24716200

$TS^{a}_{10\text{-}11}$

E(M06-2X-SMD/BS1) = -932.8776569 au
H(M06-2X-SMD/BS1) = -932.534214 au
G(M06-2X-SMD/BS1) = -932.616085 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1219.556617 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -933.2632728 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -933.3149892 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1219.495233 au

I	0.73476800	-1.62053000	0.20287100
C	-1.37625100	-1.72650700	0.05565000
C	-4.16292500	-1.85745700	-0.16099400
C	-1.97428800	-1.97643500	-1.18415600
C	-2.18065000	-1.52344200	1.18286100
C	-3.56916100	-1.59095700	1.07272500
C	-3.36287000	-2.04963500	-1.28826800
H	-1.35642800	-2.12588200	-2.06509400
H	-1.72235900	-1.32273400	2.14742200
H	-4.18621100	-1.43716300	1.95320800
H	-3.81977000	-2.25376200	-2.25222800
H	-5.24396800	-1.91241100	-0.24495400
O	2.23556800	1.80168500	0.88479700
C	1.08296700	1.60488900	0.55252200
C	-1.64076400	1.76044500	-0.24246400
C	-0.01430700	1.54737700	1.55685100
C	0.68778400	1.49638300	-0.88249100
C	-0.60656700	1.61018800	-1.24387600
C	-1.29842400	1.63945400	1.16927400
H	0.27603200	1.48206900	2.60120900
H	1.50465200	1.34413200	-1.58291400
H	-0.91297700	1.57608400	-2.28488600
H	-2.11469300	1.64039000	1.88607700
C	-3.05507500	1.58914200	-0.65126500
H	-3.74771200	1.96227900	0.10656700
H	-3.22531700	0.50718300	-0.75919400
H	-3.24564500	2.05552600	-1.61975400
O	3.18197800	-0.14746600	-1.57433500
C	3.72285600	-0.40120800	-0.48006800
O	3.26937700	-1.15570100	0.43520200
C	5.06078600	0.27959100	-0.16517800
H	4.85064100	1.21024800	0.37372800

H	5.59902400	0.52989900	-1.08292600
H	5.68574400	-0.34809500	0.47529000
O	-1.77828900	3.87013000	-0.28825900
H	-2.39569200	4.07314700	0.44125600
C	-0.55224500	4.55659600	-0.04441800
H	-0.74625900	5.62906300	0.04517900
H	-0.07009600	4.20070800	0.87419000
H	0.09404900	4.37767600	-0.90383000

11

E(M06-2X-SMD/BS1) = -461.0727057 au
H(M06-2X-SMD/BS1) = -460.895685 au
G(M06-2X-SMD/BS1) = -460.940495 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -461.2638299 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -461.2557254 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -461.2695839 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -461.2476295 au

O	3.35024600	-0.26490100	-0.12772900
C	2.13476800	-0.13662300	-0.09609400
C	-0.77921300	0.20199100	0.14036300
C	1.23843200	-1.28756300	0.15139200
C	1.48510800	1.17136200	-0.33176700
C	0.15956300	1.31094000	-0.25603400
C	-0.08648100	-1.13640300	0.23254400
H	1.71617900	-2.25790500	0.25328000
H	2.13976800	2.00078600	-0.58314800
H	-0.31946000	2.26873800	-0.44944100
H	-0.72464800	-1.99878900	0.41479400
C	-1.36882300	0.55239500	1.51802600
H	-0.55856000	0.69413100	2.23822200
H	-2.01850500	-0.24746000	1.88494300
H	-1.94796100	1.47881400	1.44684100
O	-1.77249100	0.18493600	-0.88409000
C	-2.95898100	-0.53249800	-0.60104800
H	-2.76241400	-1.56154900	-0.27686100
H	-3.57097300	-0.03189500	0.15816100
H	-3.52170100	-0.56675000	-1.53652900

12

E(M06-2X-SMD/BS1) = -1046.229942 au
H(M06-2X-SMD/BS1) = -1045.874489 au
G(M06-2X-SMD/BS1) = -1045.958391 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1332.849597 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -1046.660987 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -1046.701626 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1332.907733 au

I	-0.60146000	0.20943600	0.40432600
C	-2.63660100	-0.03578400	-0.11928900
C	-5.31704300	-0.30760400	-0.76785200
C	-3.46671900	-0.79450300	0.70699100

C	-3.12835600	0.58974400	-1.26331300
C	-4.47921500	0.45183300	-1.58229400
C	-4.81197900	-0.93236600	0.37255600
H	-3.06354900	-1.27727600	1.59293300
H	-2.47047600	1.17532700	-1.89813000
H	-4.87280800	0.93543400	-2.47089400
H	-5.46526700	-1.52374200	1.00651800
H	-6.36706400	-0.41389700	-1.02205800
O	-0.20102800	-2.48441300	2.21639200
C	0.42584300	-2.53030100	1.17456100
C	1.89444500	-2.57907800	-1.33452700
C	1.68920500	-3.26344300	1.03572800
C	-0.11422800	-1.85763600	-0.09173300
C	0.73332200	-1.90336500	-1.30752500
C	2.36432400	-3.26874600	-0.12659900
H	2.05766600	-3.76712300	1.92381200
H	-1.11871900	-2.24911000	-0.28969800
H	0.35143700	-1.41199100	-2.19852700
H	3.31093400	-3.80077000	-0.19701700
C	2.73594200	-2.69415500	-2.57197600
H	2.83648900	-3.74363400	-2.87159600
H	3.74781100	-2.31603900	-2.38552200
H	2.30067500	-2.13339600	-3.40226800
O	1.77212200	-0.10402700	1.01075400
C	2.69572200	0.29924000	0.23981900
O	2.58744700	1.21938900	-0.60600100
C	4.04709400	-0.38688700	0.35568600
H	4.26772600	-0.90601300	-0.58321600
H	4.06386200	-1.10268900	1.17813600
H	4.82486500	0.36853800	0.50087900
H	1.58741200	2.36214400	-0.22600300
O	0.89904100	3.03876500	0.10991300
C	1.33570900	4.28217800	-0.05139500
O	2.40632700	4.56168900	-0.55122400
C	0.34702600	5.30158300	0.45334600
H	-0.60180600	5.18964700	-0.07938900
H	0.15139400	5.13130900	1.51599100
H	0.73855600	6.30770400	0.30499900

$H(OAc)_2^-$
E(M06-2X-SMD/BS1) = -228.493728 au
H(M06-2X-SMD/BS1) = -228.439037 au
G(M06-2X-SMD/BS1) = -228.471619 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -228.7188005 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -457.6183305 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -457.7029897 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -457.6518154 au

O	-1.14730100	0.37114500	-0.81126300
C	-1.94460600	-0.17860700	0.03208800
O	-1.65959400	-1.07932500	0.82689800

C	-3.36219800	0.39155400	0.00564900
H	-3.34377200	1.43020400	0.35338800
H	-4.02993000	-0.18761200	0.64631500
H	-3.74790000	0.40079800	-1.01824500
O	1.63232500	1.14192700	0.73742800
C	1.95133100	0.18564700	0.04456800
O	1.15061300	-0.46868900	-0.75294700
C	3.36650400	-0.35995500	0.03097300
H	3.99847700	0.19959600	0.72158100
H	3.77837200	-0.29304500	-0.98075800
H	3.35907200	-1.41767700	0.31083100
H	0.11115100	-0.08455300	-0.71371000

13

E(M06-2X-SMD/BS1) = -588.6909001 au
H(M06-2X-SMD/BS1) = -588.461397 au
G(M06-2X-SMD/BS1) = -588.519524 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -875.2015964 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -588.885994 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -588.982758 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -875.102920 au

I	1.00919900	-1.42348300	-0.10320400
C	-0.99719200	-0.96210300	0.20441100
C	-3.63051000	-0.23713600	0.56203800
C	-1.87620900	-1.07700900	-0.87263000
C	-1.39825700	-0.49397100	1.45523200
C	-2.73317500	-0.13116600	1.62426800
C	-3.20561400	-0.70927400	-0.68016600
H	-1.53229200	-1.44087000	-1.83486200
H	-0.69007800	-0.40984100	2.27233400
H	-3.06737600	0.23568400	2.58924600
H	-3.90627100	-0.78973800	-1.50483700
H	-4.66783600	0.04971000	0.70281800
O	3.33582200	1.21611400	0.67500900
C	2.16052000	1.33004000	0.38863000
C	-0.39767100	2.06539000	-0.68756300
C	1.18173900	2.05273500	1.21543800
C	1.60890400	0.70728800	-0.88428900
C	0.40439100	1.28232900	-1.44887400
C	-0.01111800	2.39019900	0.69325400
H	1.48647100	2.34364100	2.21530700
H	2.38850600	0.39047300	-1.57574600
H	0.12676200	1.01374900	-2.46361300
H	-0.72572500	2.95582900	1.28657200
C	-1.68979600	2.62472600	-1.18904200
H	-1.68256400	3.71942700	-1.13490900
H	-2.51152900	2.27814900	-0.54882500
H	-1.88828400	2.31718000	-2.21797200

14

E(M06-2X-SMD/BS1) = -588.6775583 au
H(M06-2X-SMD/BS1) = -588.448092 au
G(M06-2X-SMD/BS1) = -588.507346 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -875.1519772 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -588.8786016 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -588.9707294 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -875.090720 au

I	1.72806700	-1.16804100	-0.19111800
C	1.37212700	0.86226200	-0.22025500
C	0.74553400	3.53740100	-0.17806100
C	1.94940100	1.66773600	0.76505700
C	0.49080000	1.35836400	-1.18459300
C	0.18054100	2.71480800	-1.15155000
C	1.62529300	3.01970900	0.77459900
H	2.62666300	1.24763500	1.50048900
H	0.05638400	0.70256400	-1.93188700
H	-0.50324600	3.12473900	-1.88714800
H	2.05980800	3.66848400	1.52762900
H	0.49906200	4.59420900	-0.16036100
O	0.19084400	-1.60447700	1.02399200
C	-1.02749100	-1.07744000	0.65098800
C	-3.53919300	-0.04131400	0.01559400
C	-1.81745000	-1.73006000	-0.29704200
C	-1.46080000	0.09600600	1.26508800
C	-2.72062300	0.59926600	0.94911100
C	-3.06761400	-1.21041300	-0.60149700
H	-1.44621900	-2.62979000	-0.77911900
H	-0.81473500	0.59455700	1.98147000
H	-3.06739100	1.50990700	1.42954200
H	-3.69295200	-1.71514200	-1.33312000
C	-4.90439500	0.49651700	-0.31966400
H	-5.68580000	-0.11754400	0.14244100
H	-5.07767900	0.48413900	-1.40004900
H	-5.02498400	1.52116000	0.04081100

$TS_{3\text{-}7}$
E(M06-2X-SMD/BS1) = -1046.216578 au
H(M06-2X-SMD/BS1) = -1045.862692 au
G(M06-2X-SMD/BS1) = -1045.948165 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1332.942827 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -1046.652466 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -1046.685517 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1332.904349 au

I	-0.04249600	0.84426200	-0.51381400
C	-1.20297000	-0.15820200	0.89929800
C	-2.78899500	-1.35382900	2.79670200
C	-2.17750900	-1.05821600	0.47514900
C	-0.99775500	0.16547100	2.23813000
C	-1.80832200	-0.44546800	3.19215800
C	-2.97327000	-1.65815400	1.44763700

H	-2.29026900	-1.29139700	-0.57601500
H	-0.22532900	0.86975700	2.52971000
H	-1.66801000	-0.21115900	4.24227100
H	-3.73942900	-2.36534500	1.14692500
H	-3.41443000	-1.82978500	3.54543900
O	1.36478100	-2.12077300	1.25318200
C	2.04603700	-1.05460700	0.87439900
C	3.56610900	1.25438500	0.17428500
C	2.40665000	-0.79474000	-0.46866700
C	2.43830100	-0.11196100	1.85597700
C	3.16996400	1.00572400	1.50646300
C	3.18836200	0.32989700	-0.78839600
H	2.14288300	-1.51466100	-1.23421500
H	2.15627900	-0.29914900	2.88781000
H	3.45774500	1.71365300	2.28088500
H	3.47861700	0.48440600	-1.82495600
C	4.37931400	2.47588800	-0.16457800
H	3.84293800	3.39420600	0.09878300
H	4.60873800	2.51136700	-1.23291600
H	5.32577900	2.48573800	0.38716700
O	-0.23946700	-1.85828500	-1.58440600
C	0.01073600	-3.07884900	-1.50483300
O	0.74126500	-3.62994800	-0.62107500
C	-0.62317500	-4.01911500	-2.52145300
H	-0.90422400	-3.48026000	-3.42810000
H	-1.52913800	-4.45109600	-2.08089500
H	0.05328300	-4.84192400	-2.76397200
O	-1.24027100	2.47106100	-0.41803700
C	-2.45484300	2.36629900	-1.01036100
O	-2.84152900	1.36056500	-1.55023600
C	-3.21759700	3.65522200	-0.88120700
H	-3.34954400	3.89627900	0.17684700
H	-2.64931400	4.46548900	-1.34505700
H	-4.18725400	3.54859700	-1.36655700
H	1.09850100	-2.73002600	0.42933800

6 in CH_2Cl_2
E(M06-2X-SMD/BS1) = -346.6359799 au
H(M06-2X-SMD/BS1) = -346.494144 au
G(M06-2X-SMD/BS1) = -346.534369 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -346.7807822 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -346.7754508 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -346.7886035 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -346.7665003 au

O	-2.79768200	-0.09661700	0.00203500
C	-1.43891700	-0.01967300	0.00104800
C	1.37614600	0.01266300	-0.00325000
C	-0.72363000	-1.21996800	-0.00029000
C	-0.75274000	1.19323100	-0.00024800
C	0.64170700	1.19871900	-0.00261900

C	0.66485100	-1.19416000	-0.00271100
H	-1.26983000	-2.15813700	-0.00099400
H	-1.30745500	2.12869000	-0.00095400
H	1.16582700	2.15120100	-0.00462700
H	1.21208600	-2.13411200	-0.00500900
C	2.88390700	0.01809700	0.00359500
H	3.27466000	1.03378900	-0.10272600
H	3.28739100	-0.58727900	-0.81507800
H	3.27866300	-0.39689400	0.93789000
H	-3.16782800	0.80222000	0.00206600

3 in CH_2Cl_2
E(M06-2X-SMD/BS1) = -699.6054955 au
H(M06-2X-SMD/BS1) = -699.392300 au
G(M06-2X-SMD/BS1) = -699.457479 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -986.1834796 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -699.9089884 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -699.9290882 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -986.1604324 au

I	0.48967100	-0.73258200	-0.20423700
C	-0.63583200	1.04211700	-0.13728400
C	-2.14743800	3.34445400	-0.03963300
C	-0.35944700	1.98073300	0.84962000
C	-1.64652600	1.21794800	-1.07533000
C	-2.40637100	2.38535200	-1.01647500
C	-1.12771400	3.14278600	0.88865200
H	0.43505600	1.81510400	1.56837200
H	-1.84448700	0.46515700	-1.83089300
H	-3.19775600	2.54237300	-1.74240300
H	-0.92975300	3.88570400	1.65463600
H	-2.74277100	4.25112000	-0.00066800
O	2.10317400	0.64283400	-0.00278300
C	3.25635300	0.00897400	0.04325100
O	3.34009200	-1.20813000	-0.03630600
C	4.44249600	0.92548300	0.19930300
H	4.33883600	1.50384500	1.12149800
H	4.47099400	1.63116500	-0.63549100
H	5.36235400	0.34157500	0.22622200
O	-1.33450100	-1.71937300	-0.51996700
C	-2.18701000	-1.76614300	0.50110300
O	-1.96529800	-1.27420100	1.58883300
C	-3.46573300	-2.48005400	0.13889600
H	-3.98913000	-1.90579900	-0.63180600
H	-3.24036800	-3.46577100	-0.27579500
H	-4.09993800	-2.57657100	1.02008500

$(HOAc)_2$ in CH_2Cl_2
E(M06-2X-SMD/BS1) = -458.0013885 au
H(M06-2X-SMD/BS1) = -457.863122 au
G(M06-2X-SMD/BS1) = -457.911089 au

E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -458.2142346 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -458.1871062 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -458.195054 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -458.2046496 au

O	-1.24208200	-1.06742700	0.00001400
C	-1.93317600	-0.05559300	-0.00002200
O	-1.43114600	1.16275600	-0.00007100
C	-3.43093000	-0.08299300	0.00008300
H	-3.78513000	-1.11269500	-0.00071600
H	-3.80304800	0.44470200	-0.88249100
H	-3.80279500	0.44315400	0.88370000
H	-0.43291600	1.11450800	-0.00008900
O	1.24209300	1.06743800	-0.00017600
C	1.93317400	0.05559600	-0.00007800
O	1.43114200	-1.16275300	0.00006500
C	3.43092600	0.08297700	0.00006400
H	3.78513300	1.11267600	-0.00141300
H	3.80310300	-0.44535100	-0.88210100
H	3.80272100	-0.44254000	0.88408900
H	0.43290800	-1.11450300	0.00007600

MeOH in CH_2Cl_2
E(M06-2X-SMD/BS1) = -115.658476 au
H(M06-2X-SMD/BS1) = -115.602322 au
G(M06-2X-SMD/BS1) = -115.629277 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -115.7203344 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -115.7121572 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -115.7168258 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -115.7150382 au

O	-0.74649600	0.12372700	0.00000000
H	-1.12934400	-0.76641200	0.00000000
C	0.66051200	-0.01939800	0.00000000
H	1.08661700	0.98685200	-0.00000100
H	1.02581200	-0.54693300	0.89116600
H	1.02581200	-0.54693400	-0.89116500

10 in CH_2Cl_2
E(M06-2X-SMD/BS1) = -817.2219331 au
H(M06-2X-SMD/BS1) = -816.934891 au
G(M06-2X-SMD/BS1) = -817.008855 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1103.837715 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -817.5729873 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -817.6032248 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1103.803301 au

I	0.39444200	-0.83076600	-0.15332000
C	2.41772600	-0.14210300	-0.11047700
C	5.07394900	0.67428500	-0.03184900
C	2.99422900	0.21876000	1.10892000
C	3.16139200	-0.10017200	-1.28882500
C	4.49512200	0.30729600	-1.24487700

C	4.32389000	0.63333400	1.14368500
H	2.40459800	0.18300000	2.02196500
H	2.70813200	-0.38124300	-2.23538500
H	5.07842200	0.34084500	-2.16004900
H	4.77557000	0.91776900	2.08918700
H	6.11120900	0.99320000	-0.00111500
O	-0.70374600	0.57125600	2.61096300
C	-1.16714200	1.06670600	1.60028200
C	-2.19653600	2.29273300	-0.82476500
C	-2.51649000	1.64101900	1.54047300
C	-0.31919500	1.17353800	0.33050700
C	-0.94877500	1.79670700	-0.85915000
C	-2.98164900	2.20165800	0.41131700
H	-3.11189200	1.57422700	2.44544700
H	0.62683600	1.66151800	0.58726600
H	-0.34128500	1.87683400	-1.75719200
H	-3.98868300	2.61323200	0.39041300
C	-2.83663800	2.96430100	-2.00528500
H	-3.12315000	3.99290600	-1.75840900
H	-3.75210200	2.43581900	-2.29537600
H	-2.16248800	2.98712200	-2.86470400
O	-1.94387800	-0.98448000	-0.02298100
C	-2.32485800	-2.20268900	-0.21153600
O	-1.56195300	-3.13480900	-0.48162500
C	-3.82177600	-2.42403200	-0.07279200
H	-4.35638000	-1.77369600	-0.77154900
H	-4.13840800	-2.14837200	0.93782300
H	-4.07870300	-3.46632000	-0.26700300

$TS_{10\text{-}11}$ in CH_2Cl_2
E(M06-2X-SMD/BS1) = -932.8867295 au
H(M06-2X-SMD/BS1) = -932.543233 au
G(M06-2X-SMD/BS1) = -932.624774 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1219.56349 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -933.2977176 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -933.3285828 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1219.527946 au

I	0.46061100	-1.27449200	-0.32696700
C	2.42271900	-0.50293000	-0.31008200
C	4.96904000	0.61656700	-0.26866400
C	3.48615800	-1.22761700	0.22969500
C	2.62205200	0.77977700	-0.82727300
C	3.90084500	1.33571400	-0.80260200
C	4.76061000	-0.66275700	0.24522000
H	3.32358700	-2.22293200	0.63191900
H	1.78050200	1.33086800	-1.24116600
H	4.06097500	2.33149100	-1.20532400
H	5.59102300	-1.22529000	0.66129100
H	5.96367700	1.05142400	-0.25403200
O	-1.29880000	-1.23293400	2.99289200

C	-1.20669100	-0.27860100	2.24863300
C	-0.98299500	2.28690000	1.05983100
C	-2.38433400	0.37116900	1.62895900
C	0.12412700	0.36348400	1.98271300
C	0.18563400	1.65574600	1.51902700
C	-2.26048100	1.58844100	1.07338000
H	-3.32871400	-0.15814000	1.69145300
H	0.98580800	-0.12605200	2.42801300
H	1.13140300	2.18495500	1.46985400
H	-3.11517700	2.09738000	0.63817700
C	-0.96471400	3.73024900	0.71945800
H	-1.13729200	4.29167000	1.64984300
H	-1.76541000	3.99312400	0.02565900
H	0.00563600	4.03386200	0.32061900
O	-2.13844200	-1.88521800	-0.21000200
C	-2.86996500	-1.22034100	-0.99145100
O	-2.54479300	-0.18865300	-1.63434000
C	-4.31841300	-1.68380700	-1.14642400
H	-4.96353800	-1.03411800	-0.54294100
H	-4.44452000	-2.71319800	-0.80611200
H	-4.63989900	-1.58831400	-2.18679600
H	-1.30355900	0.88068800	-1.38026900
O	-0.77036700	1.72669700	-1.36630600
C	-1.43545100	2.60122200	-2.25047500
H	-2.47048500	2.80309400	-1.93841000
H	-0.88924300	3.54875900	-2.28134100
H	-1.46681900	2.19037800	-3.26878900

12 in CH_2Cl_2
E(M06-2X-SMD/BS1) = -1046.23058 au
H(M06-2X-SMD/BS1) = -1045.874138 au
G(M06-2X-SMD/BS1) = -1045.960405 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1332.952038 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -1046.662719 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -1046.69881 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1332.911186 au

I	0.60444200	0.43217600	-0.06951600
C	2.70046400	0.20479000	0.17900100
C	5.44873800	-0.02275900	0.46986100
C	3.46873900	-0.24586900	-0.89516000
C	3.28976400	0.54507500	1.39543100
C	4.67300200	0.43155300	1.53453900
C	4.84823000	-0.36414500	-0.74188300
H	2.98993100	-0.51189200	-1.83416500
H	2.68234900	0.89335300	2.22547400
H	5.14138500	0.69437800	2.47797100
H	5.45308100	-0.71804500	-1.57100900
H	6.52453400	-0.11228400	0.58432400
O	0.36693200	-1.66404600	-2.56503800
C	-0.22906900	-2.04935600	-1.57635600

C	-1.62404500	-2.91218600	0.82162600
C	-1.44205600	-2.87045500	-1.64708200
C	0.30142900	-1.73003600	-0.17500500
C	-0.50255200	-2.18952300	0.98215000
C	-2.08181200	-3.25693900	-0.52991700
H	-1.80153100	-3.11947000	-2.64027800
H	1.34000400	-2.07273900	-0.10875500
H	-0.13466600	-1.94495000	1.97501600
H	-2.99067200	-3.85026700	-0.60818800
C	-2.44217400	-3.40709300	1.97835900
H	-2.49196000	-4.50199400	1.97898400
H	-3.47168700	-3.03852000	1.90053500
H	-2.02546700	-3.07455800	2.93174800
O	-1.75330500	0.12235500	-0.54313500
C	-2.57269300	0.20351500	0.42715300
O	-2.33039900	0.76416700	1.52217500
C	-3.95436400	-0.37587100	0.20166100
H	-4.39083100	-0.70578900	1.14675600
H	-3.93372700	-1.19142300	-0.52379900
H	-4.58161100	0.42843800	-0.19975900
H	-1.65711900	2.14466600	1.13546800
O	-1.21146700	2.97527500	0.75392200
C	-1.99965200	3.49664200	-0.18479700
O	-3.10255700	3.06644900	-0.45159300
C	-1.35995000	4.67385500	-0.87304000
H	-1.04936100	5.41572500	-0.13230500
H	-0.46314100	4.34026800	-1.40455700
H	-2.06057500	5.11900000	-1.57899900

13 in CH_2Cl_2
E(M06-2X-SMD/BS1) = -588.684380 au
H(M06-2X-SMD/BS1) = -588.454789 au
G(M06-2X-SMD/BS1) = -588.512923 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -875.1949576 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -588.8873633 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -588.9772252 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -875.1035727 au

I	1.00858300	-1.42889900	-0.09654000
C	-0.99708000	-0.96080000	0.20171100
C	-3.63243300	-0.23411200	0.54446500
C	-1.87125400	-1.07670400	-0.87937300
C	-1.40494300	-0.48997500	1.45013100
C	-2.74044300	-0.12669700	1.61121900
C	-3.20144400	-0.70863700	-0.69453700
H	-1.52453200	-1.44481100	-1.83901400
H	-0.70240400	-0.40625300	2.27215500
H	-3.08012700	0.24080900	2.57398000
H	-3.89822900	-0.79164000	-1.52216800
H	-4.67059100	0.05213000	0.67975700
O	3.34339100	1.22079500	0.65209100

C	2.16718900	1.33646500	0.37476700
C	-0.40111800	2.06668300	-0.67294000
C	1.18865800	2.04099200	1.21958300
C	1.61239100	0.73448300	-0.90575000
C	0.40509800	1.30105400	-1.45311100
C	-0.01060000	2.37493100	0.71037500
H	1.49961600	2.32141800	2.22053300
H	2.38615600	0.40640800	-1.59765600
H	0.12376200	1.05146900	-2.47155000
H	-0.72635600	2.92717400	1.31457000
C	-1.69727700	2.62487100	-1.16095100
H	-1.70072400	3.71771500	-1.07788000
H	-2.51509500	2.25329400	-0.52920900
H	-1.89393600	2.34227500	-2.19716600

16

E(M06-2X-SMD/BS1) = -703.8751645 au
H(M06-2X-SMD/BS1) = -703.8751645 au
G(M06-2X-SMD/BS1) = -703.666839 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -990.4408007 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -704.1933417 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -704.2158853 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -990.4145116 au

I	0.26172800	-0.92038900	-0.61677400
C	2.16133700	-0.03780400	-0.06965600
C	4.64041500	1.05786300	0.59162600
C	2.74110900	-0.31888800	1.16989400
C	2.82203800	0.79126800	-0.97703700
C	4.06315400	1.33764100	-0.64552900
C	3.97915500	0.23053400	1.49993900
H	2.22660700	-0.96514800	1.87765500
H	2.37280800	1.01300400	-1.94199300
H	4.57560600	1.98332600	-1.35271200
H	4.42918300	0.01027500	2.46359800
H	5.60535400	1.48395600	0.84925200
O	-1.62093600	-1.18549700	2.12615800
C	-1.84837400	-0.23038700	1.40332800
C	-2.31150200	2.19069200	-0.13085600
C	-3.19819000	0.32728100	1.22807300
C	-0.70047000	0.51557600	0.72451100
C	-1.04864900	1.74064500	-0.03571800
C	-3.39828000	1.45499200	0.52633000
H	-4.01011000	-0.20861900	1.71031700
H	0.09511300	0.69480600	1.45352900
H	-0.22776800	2.28489300	-0.49779900
H	-4.40395400	1.85730000	0.42269000
C	-2.67271100	3.44287700	-0.87722600
H	-3.15907100	4.16419900	-0.21055400
H	-3.38352600	3.22008600	-1.68145400
H	-1.78927700	3.91387700	-1.31506400

O	-1.86631200	-1.34706800	-0.85327700
C	-2.15673900	-2.69126600	-0.65327400
H	-3.08483600	-2.97035200	-1.17677800
H	-1.36795400	-3.36789300	-1.03822900
H	-2.28552300	-2.93873400	0.41708000

17

E(M06-2X-SMD/BS1) = -932.895657 au
H(M06-2X-SMD/BS1) = -932.551897 au
G(M06-2X-SMD/BS1) = -932.634651 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1219.570779 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -933.2904318 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -933.3272562 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1219.52836 au

I	-0.35861900	0.48923400	-0.10962900
C	-2.46520300	0.31968500	-0.08687300
C	-5.22867800	0.12507800	-0.05510500
C	-3.13781400	0.34251300	1.13559500
C	-3.15469200	0.20501400	-1.29286700
C	-4.54587900	0.10930800	-1.26983500
C	-4.52696900	0.23898100	1.14518900
H	-2.58352100	0.43167000	2.06556500
H	-2.61716500	0.18858300	-2.23592600
H	-5.09297600	0.01908400	-2.20303600
H	-5.06008700	0.25184600	2.09065300
H	-6.31142500	0.04819200	-0.04248500
O	0.62623000	-0.93353000	2.70795500
C	0.86919300	-1.58997200	1.71229500
C	1.37594000	-3.16375300	-0.67728500
C	2.05226400	-2.45124000	1.59296100
C	-0.10073100	-1.59081000	0.52835000
C	0.25749300	-2.41956900	-0.64720000
C	2.28055200	-3.16750000	0.47899300
H	2.73251000	-2.45944700	2.43876900
H	-1.10764200	-1.80929100	0.89911200
H	-0.43865800	-2.42294000	-1.48241600
H	3.17198900	-3.78748200	0.40917400
C	1.75407000	-4.01069200	-1.85706300
H	1.86853700	-5.05974500	-1.56194200
H	2.71861500	-3.68416200	-2.26400400
H	1.00343700	-3.94842000	-2.64843800
O	1.17857100	2.88918800	-0.85536100
C	2.14573900	3.22506200	-0.14690400
O	2.85423400	2.43845200	0.56658000
C	2.55721000	4.69184700	-0.09365900
H	2.50334500	5.05051900	0.93909300
H	1.91373700	5.30495300	-0.72667600
H	3.59726200	4.79498700	-0.41852500
O	2.12447100	0.13406900	0.01643500
C	2.74417700	-0.12636400	-1.22572200

H	2.00227000	-0.21669400	-2.03127700
H	3.43708600	0.68293400	-1.48654900
H	3.30819100	-1.06702800	-1.17479600
H	2.43322300	1.10210500	0.31392500

TS_{17-11}

E(M06-2X-SMD/BS1) = -1048.563751 au
H(M06-2X-SMD/BS1) = -1048.162689 au
G(M06-2X-SMD/BS1) = -1048.256265 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1335.299777 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -1049.027873 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -1049.061108 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1335.261346 au

I	0.74967100	-0.52519700	-0.96528500
C	2.78386400	-0.45779400	-0.46372000
C	5.46267600	-0.34922400	0.26419400
C	3.38447600	-1.57551200	0.11732900
C	3.50631800	0.71887100	-0.67213200
C	4.85014600	0.76547300	-0.30832100
C	4.72995200	-1.51539600	0.47681100
H	2.81169100	-2.48181700	0.28551100
H	3.02664700	1.58690700	-1.11395800
H	5.41721300	1.67671100	-0.47196100
H	5.20225600	-2.38337200	0.92647700
H	6.50981800	-0.30686700	0.54709800
O	1.85864900	0.35268200	2.35049400
C	0.86478600	0.86056600	1.86496000
C	-1.61720000	2.10168100	1.30681100
C	-0.38288800	0.06416100	1.64018700
C	0.80642100	2.29593400	1.50441000
C	-0.38434000	2.87380600	1.26420200
C	-1.58329500	0.70537300	1.43955500
H	-0.35911200	-1.00169600	1.84402600
H	1.73823300	2.85255900	1.51639900
H	-0.46411700	3.93526500	1.05168800
H	-2.50374200	0.13297500	1.36853800
C	-2.90903500	2.82669100	1.32812900
H	-3.10759400	3.11352200	2.37206400
H	-3.73216800	2.19135400	0.99433100
H	-2.86316800	3.74477800	0.73869100
O	-2.00231600	-0.37310800	-1.37816500
H	-1.74923700	1.29450200	-1.28558500
O	-1.70279300	2.28175800	-1.29117800
C	-2.89841500	2.71855300	-1.90019400
H	-3.79136800	2.27782700	-1.43434600
H	-2.96096200	3.80624000	-1.79946600
H	-2.92014100	2.47597000	-2.97277900
H	-2.63390300	-0.84685400	-0.69670000
C	-2.40866500	-0.75142800	-2.67797100
H	-2.29451700	-1.83214600	-2.83417300

H	-3.45632200	-0.48241000	-2.86728700
H	-1.78059600	-0.23072600	-3.40861200
O	-3.65423000	-1.54505600	0.10827500
C	-3.10142900	-2.39067100	0.89240200
O	-1.88909000	-2.45649400	1.15085500
C	-4.06317100	-3.37821700	1.55031700
H	-4.60232000	-3.93900700	0.78021200
H	-3.53111700	-4.07291400	2.20268100
H	-4.81099100	-2.83080500	2.13320100

H(OMe)(OAc)
E(M06-2X-SMD/BS1) = -344.176941 au
H(M06-2X-SMD/BS1) = -344.063939 au
G(M06-2X-SMD/BS1) = -344.108754 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -344.3536154 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -344.243988 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -344.327535 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -344.268711 au

O	2.12034400	-0.61217200	-0.44511900
H	1.14231400	-0.76821000	-0.30336300
C	2.45428000	0.44279500	0.41384600
H	1.74876600	1.27978500	0.32531300
H	2.47801900	0.13931300	1.47587600
H	3.45882300	0.80482300	0.16098400
O	-0.44701300	-1.00729900	0.08597200
C	-1.11751200	0.06044500	-0.05343200
O	-0.68287000	1.18787200	-0.35267400
C	-2.62825600	-0.09489100	0.18655000
H	-2.80719700	-0.44311200	1.20966400
H	-3.15900500	0.84698300	0.03018400
H	-3.03647300	-0.85688500	-0.48586900

TS′$_{10\text{-}11}$
E(M06-2X-SMD/BS1) = -932.8847689 au
H(M06-2X-SMD/BS1) = -932.541495 au
G(M06-2X-SMD/BS1) = -932.623487 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -1219.562510 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -933.290335 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -933.3271905 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -1219.515594 au

I	0.38010100	-1.57428500	-0.02618400
C	-1.66508300	-1.22894600	0.34148800
C	-4.35422100	-0.75696200	0.93031500
C	-2.66078100	-1.95116900	-0.32276300
C	-2.01665100	-0.24853400	1.27924000
C	-3.36204600	-0.02194300	1.57478600
C	-4.00148000	-1.71675000	-0.02166500
H	-2.39118300	-2.70399800	-1.05752600
H	-1.23518700	0.32157800	1.77740800
H	-3.63014100	0.73382600	2.30757000

H	-4.77297200	-2.28793600	-0.52970900
H	-5.40031500	-0.58108900	1.16161600
O	1.95019200	2.59280200	-0.93860600
C	0.79645300	2.22807700	-0.84236100
C	-1.98475300	1.78629800	-1.06333600
C	-0.16667800	2.90873100	0.06716500
C	0.24812700	1.17966000	-1.75493200
C	-1.09362800	1.04176800	-1.89422000
C	-1.49468000	2.69872000	-0.06999300
H	0.24279600	3.62607900	0.77012900
H	0.96269900	0.65930800	-2.38461600
H	-1.51741800	0.34701100	-2.61301400
H	-2.21719200	3.21626000	0.55230300
C	-3.43694000	1.65855400	-1.29442700
H	-3.66224800	2.16703500	-2.24552500
H	-4.03076500	2.11328700	-0.50141500
H	-3.71238400	0.60665700	-1.43513600
O	2.98386200	-1.72787700	-0.55905400
C	3.64656100	-0.75675100	-0.11150900
O	3.22245900	0.18377600	0.60799300
C	5.12810100	-0.69030600	-0.49184000
H	5.28372400	0.14785600	-1.18002400
H	5.46003100	-1.61169700	-0.97396300
H	5.73520900	-0.49689100	0.39727900
H	1.74094900	0.70223700	1.21756600
O	1.08883400	1.27819000	1.70244800
C	1.87971800	2.25222300	2.34669900
H	2.41946700	2.88233400	1.62451600
H	1.22393200	2.89047500	2.94732000
H	2.62077100	1.79362000	3.01486100

$TS_{5\text{-}15}$

E(M06-2X-SMD/BS1) = -461.458793 au
H(M06-2X-SMD/BS1) = -461.272297 au
G(M06-2X-SMD/BS1) = -461.322303 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -461.6506497 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -461.5794654 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -461.6754825 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -461.5524193 au

O	3.13974900	-0.78442600	-0.16576300
C	2.04483900	-0.28235700	-0.01631800
C	-0.50555700	0.87960600	0.34394900
C	1.51709700	0.72099500	-0.98125600
C	1.18140400	-0.66058300	1.13884800
C	-0.03458800	-0.10710000	1.29217300
C	0.29762700	1.25588500	-0.80470100
H	2.15989600	0.98851800	-1.81392000
H	1.58757800	-1.38711600	1.83583000
H	-0.67898200	-0.35764900	2.12863300
H	-0.11506900	1.99007900	-1.48868300

C	-1.70921600	1.65843900	0.65678300
H	-2.17315400	2.06366900	-0.24377400
H	-1.35761800	2.50999100	1.26642800
H	-2.41783300	1.09333400	1.26609000
O	-1.80881300	-0.64571800	-1.02915800
H	-1.12894700	-1.11884500	-1.54076400
C	-2.51968200	-1.60207700	-0.24958900
H	-3.05765100	-2.30447900	-0.89523000
H	-1.85259200	-2.16393200	0.41403400
H	-3.24466400	-1.04926800	0.35139900

$TS'_{5\text{-}15}$

E(M06-2X-SMD/BS1) = -461.457730 au
H(M06-2X-SMD/BS1) = -461.270662 au
G(M06-2X-SMD/BS1) = -461.318248 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -461.6476261 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -461.5783354 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -461.6739376 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -461.5500028 au

O	2.26906000	1.50675400	0.25149600
C	1.17036900	1.01409700	0.12428600
C	-1.54980700	0.22801200	0.17706400
C	0.28855700	1.30253100	-1.03099700
C	0.61857200	0.09075500	1.17648300
C	-0.73654500	-0.17708100	1.23256200
C	-1.00159600	0.93193700	-0.98260300
H	0.71133600	1.86421800	-1.85745400
H	1.28108700	-0.13251400	2.00748300
H	-1.16181300	-0.72928400	2.06300000
H	-1.68572100	1.16638400	-1.79230300
C	-3.00415000	-0.04125700	0.17897300
H	-3.26054300	-0.62314800	-0.71652600
H	-3.54349500	0.91079600	0.08393400
H	-3.32892400	-0.56816100	1.07583700
O	1.49468000	-1.48215300	-0.03881700
H	1.75771900	-2.07432000	0.69123800
C	0.56732900	-2.17618300	-0.87254900
H	0.88628600	-3.21386600	-0.99697000
H	-0.44243900	-2.16381700	-0.44097400
H	0.56021500	-1.66996200	-1.83800200

$TS_{14\text{-}5}$

E(M06-2X-SMD/BS1) = -588.6744036 au
H(M06-2X-SMD/BS1) = -588.447217 au
G(M06-2X-SMD/BS1) = -588.501736 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -875.6492756 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -588.889307 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -588.975484 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -875.093583 au

I	2.31035800	-0.25648900	-0.11130900

C	0.77022500	1.08459300	-0.22976300
C	-1.48886100	2.67237300	-0.26691400
C	0.54537500	1.97680500	0.83203000
C	-0.11199200	0.98909000	-1.31503000
C	-1.25338400	1.78462200	-1.31646200
C	-0.58561100	2.78017800	0.79484100
H	1.24159700	2.02818100	1.66242300
H	0.09403100	0.30891400	-2.13462300
H	-1.95480400	1.71277900	-2.14147900
H	-0.77405900	3.47786300	1.60387200
H	-2.37923400	3.29325800	-0.27864000
O	0.82701400	-1.82909100	0.71193100
C	-0.41526000	-1.50027600	0.50839300
C	-3.11095600	-0.83074400	0.10323000
C	-1.10342900	-1.95641700	-0.65568000
C	-1.10013800	-0.67466400	1.44248700
C	-2.42839900	-0.35931100	1.23836000
C	-2.43300200	-1.65178500	-0.82633400
H	-0.55544800	-2.55254900	-1.37945500
H	-0.55772200	-0.32116500	2.31404200
H	-2.95514800	0.26847400	1.95080400
H	-2.96940400	-2.01338900	-1.69892900
C	-4.53982700	-0.45919400	-0.14563200
H	-5.15634900	-1.35900500	-0.24894100
H	-4.62451000	0.09556300	-1.08754100
H	-4.94247900	0.15609700	0.66126100

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E(M06-2X-SMD/BS1) = -461.4837024 au
H(M06-2X-SMD/BS1) = -461.293902 au
G(M06-2X-SMD/BS1) = -461.340585 au
E(M06-2X-SMD/BS2// M06-2X-SMD/BS1) = -461.6731117 au
E(B3LYP/BS1//M06-2X-SMD/BS1) = -461.5791382 au
E(B3LYP-SMD/BS1//M06-2X-SMD/BS1) = -461.6852404 au
E(M06-2X/BS2//M06-2X-SMD/BS1) = -461.5648724 au

O	-3.18340500	0.27533500	0.00526800
C	-1.98320100	0.06995800	-0.00400000
C	0.86148800	-0.51057200	-0.04051600
C	-1.19844700	0.12454000	-1.26262600
C	-1.23876500	-0.23067100	1.24400200
C	0.07420700	-0.46312900	1.23358900
C	0.11316600	-0.11631400	-1.27806600
H	-1.74729900	0.36576300	-2.16773400
H	-1.81578800	-0.24935800	2.16326200
H	0.62812700	-0.68156800	2.14344400
H	0.69114200	-0.08310200	-2.19965900
C	1.58885100	-1.83489300	-0.20345300
H	2.19139500	-2.05109100	0.68263700
H	2.22269100	-1.82173800	-1.09611700
H	0.83871700	-2.62038000	-0.32456800

O	1.98559200	0.50355000	0.16999800
H	2.72163800	0.32910000	-0.46740100
C	1.63939000	1.93640300	0.18576300
H	2.54325800	2.44570600	0.51307500
H	1.32971000	2.24248600	-0.81197500
H	0.83877700	2.04117500	0.91475200

6 optimized by M06-2X/BS2
E(M06-2X-SMD/BS1) = -346.7803768 au
H(M06-2X-SMD/BS1) = -346.639346 au
G(M06-2X-SMD/BS1) = -346.679835 au

O	-2.79244200	-0.09500100	0.00257000
C	-1.43286900	-0.02134700	0.00121800
C	1.37274400	0.01347500	-0.00354600
C	-0.72012100	-1.21697700	-0.00021200
C	-0.75144400	1.18807500	-0.00052200
C	0.63931400	1.19509100	-0.00301700
C	0.66462500	-1.18982800	-0.00278500
H	-1.26130800	-2.15501200	-0.00064200
H	-1.30704300	2.11945400	-0.00121000
H	1.16084800	2.14554300	-0.00550200
H	1.21097800	-2.12681500	-0.00512900
C	2.87676400	0.01964600	0.00352400
H	3.26423500	1.03285100	-0.10088100
H	3.27642200	-0.58470300	-0.81306700
H	3.26645100	-0.39649700	0.93532300
H	-3.16512300	0.79637700	0.00257800

$(HOAc)_2$ optimized by M06-2X/BS2
E(M06-2X-SMD/BS2) = -458.2156156 au
H(M06-2X-SMD/BS2) = -458.079102 au
G(M06-2X-SMD/BS2) = -458.127664 au

O	1.23101300	1.06579300	0.00027100
C	1.91770200	0.05431900	0.00010100
O	1.40214500	-1.15382500	-0.00011700
C	3.40902200	0.07578600	-0.00012400
H	3.77074700	1.09919300	-0.00065400
H	3.77340900	-0.45474600	-0.88056000
H	3.77353500	-0.45381400	0.88082900
H	0.40199900	-1.10549200	0.00002500
O	-1.23105200	-1.06583000	-0.00018300
C	-1.91769900	-0.05432500	-0.00008700
O	-1.40213200	1.15380700	0.00024900
C	-3.40900400	-0.07572200	-0.00014100
H	-3.77074200	-1.09912100	-0.00109900
H	-3.77346700	0.45523600	-0.88028700
H	-3.77340200	0.45347500	0.88110700
H	-0.40199000	1.10535800	0.00038800

$TS_{4\text{-}5}$ optimized by M06-2X/BS2

E(M06-2X-SMD/BS2) = -1103.81784 au
H(M06-2X-SMD/BS2) = -1103.534813 au
G(M06-2X-SMD/BS2) = -1103.534813 au

I	1.41428400	0.49803400	-0.06615600
C	-0.47587400	1.30807500	-0.16441100
C	-3.08605600	2.24359700	-0.23665000
C	-0.98025400	2.05869600	0.90968700
C	-1.28336600	1.03419900	-1.27294100
C	-2.59047300	1.49584600	-1.29853200
C	-2.27574900	2.53857600	0.85862600
H	-0.35232700	2.25804300	1.76895100
H	-0.88384200	0.46974800	-2.10611900
H	-3.22267200	1.27377800	-2.14923700
H	-2.66551800	3.12516200	1.68064000
H	-4.10595200	2.60674000	-0.26402300
O	0.21762100	-1.60091800	0.65880400
C	-1.02443300	-1.50880100	0.45178300
C	-3.79968000	-1.38747700	0.04414900
C	-1.61658500	-2.03716600	-0.75189900
C	-1.88425200	-0.87993800	1.41467800
C	-3.23606400	-0.83459000	1.20701500
C	-2.96678400	-2.00628400	-0.91964800
H	-0.95501200	-2.47208600	-1.49144500
H	-1.42833700	-0.47227700	2.30827900
H	-3.88773500	-0.36527600	1.93328500
H	-3.42216000	-2.42507400	-1.80874100
C	-5.26605800	-1.32826000	-0.19580500
H	-5.66854300	-2.34296100	-0.26681500
H	-5.46566500	-0.84671700	-1.15695600
H	-5.78566600	-0.79067700	0.59391700
O	4.45944400	0.68700300	-0.49059600
C	4.49287500	-0.47985700	-0.05362900
O	3.48691200	-1.14602300	0.32165900
C	5.84015500	-1.18579200	0.05354800
H	6.64642900	-0.56503600	-0.33249400
H	5.80560200	-2.12705100	-0.49726700
H	6.03810800	-1.42753600	1.09953600

MeOH optimized by M06-2X/BS2
E(M06-2X-SMD/BS2) = -115.7205999 au
H(M06-2X-SMD/BS2) = -115.664711 au
G(M06-2X-SMD/BS2) = -115.691746 au

O	-0.74703300	0.12348100	0.00000000
H	-1.13742900	-0.75667400	0.00000000
C	0.66430800	-0.01963300	0.00000000
H	1.09080000	0.98269800	-0.00000100
H	1.01852500	-0.54803800	0.88945100
H	1.01852400	-0.54803900	-0.88945000

$TS_{10\text{-}11}$ optimized by M06-2X/BS2

E(M06-2X-SMD/BS2) = -1219.566407 au
H(M06-2X-SMD/BS2) = -1219.225376 au
G(M06-2X-SMD/BS2) = -1219.309822 au

I	0.38399900	-1.26720400	-0.31870800
C	2.36132400	-0.57620500	-0.34696000
C	4.94539400	0.41377900	-0.37690500
C	3.39019800	-1.33615900	0.19636600
C	2.60791800	0.67457800	-0.90300800
C	3.90834500	1.16584200	-0.91436900
C	4.68561700	-0.83450300	0.17673100
H	3.18517000	-2.30668200	0.62972600
H	1.79049700	1.25408600	-1.31741400
H	4.10838400	2.13847900	-1.34645100
H	5.49223800	-1.42225600	0.59679800
H	5.95691700	0.79950800	-0.38943700
O	-1.39716000	-1.19915000	2.96946500
C	-1.18434700	-0.25884900	2.24124900
C	-0.65191700	2.30417500	1.18570200
C	-2.26176100	0.52664000	1.60703400
C	0.21359000	0.23824600	2.02472900
C	0.42525900	1.53398400	1.61760300
C	-1.99187800	1.74798100	1.13244800
H	-3.25685700	0.10187100	1.61054100
H	1.00442500	-0.35896300	2.46326200
H	1.42246000	1.95352900	1.60810600
H	-2.77104200	2.36737800	0.70551300
C	-0.46900000	3.72690700	0.84092500
H	-0.69282400	4.31240200	1.74318200
H	-1.17535400	4.04346100	0.07537900
H	0.55615500	3.94276300	0.54563600
O	-2.32893900	-1.89243500	-0.28320600
C	-3.04932200	-1.13666900	-0.97634000
O	-2.66714800	-0.11151300	-1.59473900
C	-4.53654400	-1.46058600	-1.04883300
H	-5.05326400	-0.85669900	-0.29770300
H	-4.72507900	-2.51044900	-0.83211100
H	-4.94349400	-1.19668300	-2.02419900
H	-1.33334500	0.94451900	-1.47168600
O	-0.72992400	1.72646700	-1.51941800
C	-1.41724800	2.72789900	-2.23659500
H	-2.33975900	3.03683500	-1.73074500
H	-0.76544800	3.59821200	-2.32733400
H	-1.68013400	2.39119300	-3.24503700

13 optimized by M06-2X/BS2
E(M06-2X-SMD/BS2) = -875.2021149 au
H(M06-2X-SMD/BS2) = -874.973917 au
G(M06-2X-SMD/BS2) = -875.032624 au

I	0.96026600	-1.43463100	-0.11071400
C	-1.03109100	-0.94230200	0.19929100

C	-3.63941800	-0.18121300	0.56407700
C	-1.90730700	-1.03725400	-0.87344400
C	-1.41884000	-0.47917600	1.44873800
C	-2.74307300	-0.09799900	1.62241800
C	-3.22561400	-0.65026700	-0.67747200
H	-1.56981300	-1.39893800	-1.83532700
H	-0.70889700	-0.41367000	2.26203800
H	-3.06938700	0.26591100	2.58799100
H	-3.92686200	-0.71372900	-1.49934600
H	-4.66885900	0.12141600	0.70746900
O	3.35993900	1.08977000	0.68646700
C	2.19509500	1.25126700	0.40053000
C	-0.31720400	2.09738200	-0.68386500
C	1.25663200	2.02917700	1.21503900
C	1.62126200	0.65180500	-0.86855200
C	0.43896600	1.27083600	-1.43176500
C	0.08864000	2.41907300	0.68920700
H	1.57346800	2.31508700	2.20965000
H	2.38635700	0.31117400	-1.55970300
H	0.14734900	1.00182700	-2.43927400
H	-0.59347700	3.02679400	1.27408500
C	-1.58436900	2.70430100	-1.18136600
H	-1.54217100	3.79371400	-1.10806000
H	-2.41521700	2.37498300	-0.54861100
H	-1.78816200	2.41891300	-2.21180100

$H(OAc)_2^-$ optimized by M06-2X/BS2
E(M06-2X-SMD/BS2) = -457.739739 au
H(M06-2X-SMD/BS2) = -457.61856 au
G(M06-2X-SMD/BS2) = -457.667851 au

O	-1.15051000	0.36984600	-0.73960400
C	-2.01027800	-0.15942700	0.04588700
O	-1.77698500	-1.04210600	0.87484000
C	-3.42025700	0.38945900	-0.09940800
H	-3.41941800	1.45450300	0.13975000
H	-4.11399300	-0.12931200	0.55849500
H	-3.74937000	0.28917500	-1.13477600
O	1.74991600	1.08799800	0.81268000
C	2.01847400	0.17007800	0.05554700
O	1.15864800	-0.43057800	-0.71679500
C	3.41850800	-0.37837700	-0.07294000
H	4.09494100	0.13604800	0.60457800
H	3.76246900	-0.25618100	-1.10115500
H	3.41452800	-1.44681200	0.14645300
H	0.12360400	-0.05909900	-0.63681600

3 optimized by M06-2X/BS2
E(M06-2X-SMD/BS2) = -986.1846843au
H(M06-2X-SMD/BS2) = -985.973243 au
G(M06-2X-SMD/BS2) = -986.040214 au

I	0.47052900	-0.71029200	-0.22001700
C	-0.62509600	1.05959500	-0.12022400
C	-2.09267600	3.37199300	0.01449900
C	-0.65148700	1.75911000	1.07471000
C	-1.30891900	1.47712900	-1.24927800
C	-2.05365700	2.64791500	-1.16968200
C	-1.39297400	2.93155700	1.13170200
H	-0.11388100	1.39901500	1.94173700
H	-1.26697900	0.90892500	-2.16901300
H	-2.59650300	2.99322900	-2.04004500
H	-1.42847600	3.49455900	2.05539100
H	-2.67263800	4.28445400	0.06832700
O	2.10870900	0.62681500	0.02612100
C	3.25667000	-0.00198400	0.09140900
O	3.34460600	-1.21532500	0.00636300
C	4.43890000	0.90648300	0.27814800
H	4.31391400	1.47645700	1.19935100
H	4.48299800	1.61578200	-0.54890800
H	5.35565500	0.32495800	0.32044700
O	-1.35461700	-1.69481600	-0.57749200
C	-2.20332800	-1.82075000	0.42662900
O	-1.99536300	-1.38672900	1.54000800
C	-3.45959000	-2.55027100	0.03714800
H	-3.97788300	-1.97979000	-0.73486900
H	-3.20305100	-3.52232700	-0.38430400
H	-4.10492100	-2.67399800	0.90244500

12 optimized by M06-2X/BS2
E(M06-2X-SMD/BS2) = -1332.959838 au
H(M06-2X-SMD/BS2) = -1332.607242 au
G(M06-2X-SMD/BS2) = -1332.693192 au

I	0.60549600	-0.15830300	-0.87938500
C	2.52100000	-0.49419700	-0.09504700
C	5.03332800	-0.91167100	0.94758900
C	3.26098000	-1.58096300	-0.53948200
C	3.00875300	0.38917700	0.85812300
C	4.27757800	0.17079800	1.38043400
C	4.52805300	-1.78462500	-0.00833300
H	2.85766200	-2.25662500	-1.28264700
H	2.40894900	1.22821700	1.19059100
H	4.67280400	0.84909900	2.12574300
H	5.11867100	-2.62750200	-0.34371200
H	6.02184000	-1.07609800	1.35730800
O	-0.60048000	-3.16085300	-0.87236100
C	-1.16223300	-2.46482200	-0.05461400
C	-2.48547600	-0.69384800	1.82309900
C	-2.53792200	-2.69872200	0.38033500
C	-0.42877700	-1.31705900	0.63690300
C	-1.21102400	-0.42732100	1.52032600
C	-3.13983400	-1.86743300	1.24078900

H	-3.04958500	-3.54428200	-0.06161400
H	0.43943100	-1.73557400	1.15475200
H	-0.70417400	0.43727200	1.93183500
H	-4.17289500	-2.04652600	1.52193600
C	-3.29419900	0.16890800	2.74003500
H	-3.64337100	-0.40551400	3.60151400
H	-4.18130200	0.54094400	2.22086000
H	-2.71390000	1.01977000	3.09395600
O	-1.95392900	-0.04737600	-1.49188700
C	-2.83438000	0.73228400	-1.06048900
O	-2.63104900	1.88861500	-0.60182400
C	-4.27884300	0.27365900	-1.09492200
H	-4.67600200	0.26254600	-0.07788700
H	-4.37370500	-0.71613500	-1.53465200
H	-4.86933300	0.99169600	-1.66624900
H	-1.34701400	2.55334200	-0.63187600
O	-0.47947700	3.13270400	-0.77636600
C	0.31807400	3.16169600	0.26288000
O	0.05550100	2.65709900	1.33936400
C	1.62032900	3.85950300	-0.01510300
H	2.20498100	3.23943000	-0.69953600
H	1.44033200	4.81415100	-0.50890800
H	2.17834900	4.00814700	0.90544400

$TS_{3\text{-}8}$ optimized by M06-2X/BS2
E(M06-2X-SMD/BS2) = -986.1488916 au
H(M06-2X-SMD/BS2) = -985.938874 au
G(M06-2X-SMD/BS2) = -986.004769 au

I	-0.43859000	-0.21558600	-0.13354200
C	1.60142300	-0.67732700	-0.02867400
C	4.27161700	-1.32834300	0.11376900
C	2.25083700	-0.59995200	1.19861800
C	2.26056000	-1.08547200	-1.18345100
C	3.60839800	-1.40616100	-1.10538500
C	3.59734600	-0.92934100	1.26228100
H	1.71595700	-0.28409800	2.08476600
H	1.73060600	-1.14927400	-2.12529900
H	4.13798500	-1.72098600	-1.99528600
H	4.11944300	-0.87323600	2.20868400
H	5.32237100	-1.58342400	0.17011100
O	-2.47601100	-1.84139800	0.33677100
C	-3.30805900	-0.92381800	0.11810900
O	-2.98690800	0.25156100	-0.21169200
C	-4.78495500	-1.23146700	0.24820700
H	-5.26461000	-1.08643400	-0.72130800
H	-5.24046400	-0.53051300	0.94883200
H	-4.94855400	-2.25198700	0.58688900
O	-0.12232900	1.64445000	-0.74998500
C	0.27626500	2.55153800	0.17485200
O	0.48500600	2.26299000	1.31958000

C	0.41615400	3.90883100	-0.43917100
H	1.12747900	3.86048800	-1.26384300
H	-0.54733600	4.22114900	-0.84257900
H	0.75679000	4.61264100	0.31446600

TS_{1-4} optimized by M06-2X/BS2
E(M06-2X-SMD/BS2) = -1103.833138 au
H(M06-2X-SMD/BS2) = -1103.549353 au
G(M06-2X-SMD/BS2) = -1103.549353 au

I	-1.19251400	0.29325000	-0.14166900
C	0.16236900	1.85594200	0.14584900
C	2.02365900	3.85826600	0.48096700
C	0.18660300	2.91614600	-0.75523500
C	1.04928000	1.78514400	1.21529800
C	1.98585500	2.79744200	1.37750900
C	1.12817300	3.91984700	-0.58171800
H	-0.51467500	2.95199700	-1.57943600
H	1.01145000	0.95109100	1.90514300
H	2.68479100	2.75553100	2.20290800
H	1.16192800	4.75076900	-1.27456600
H	2.75546300	4.64551400	0.61153700
O	0.02923100	-0.66730400	-1.36585100
C	1.18808900	-1.16738800	-0.81262500
C	3.56975100	-2.21141000	0.19749500
C	1.15915000	-2.32236100	-0.03916900
C	2.38629600	-0.51980600	-1.07277100
C	3.56906200	-1.05172700	-0.57196400
C	2.34613900	-2.83466500	0.45671100
H	0.21063700	-2.80545200	0.16495800
H	2.38478600	0.38595100	-1.66697400
H	4.50662300	-0.54952500	-0.78033700
H	2.32647300	-3.73735800	1.05688900
C	4.84839000	-2.79439300	0.72949300
H	5.09579700	-3.72209200	0.20809800
H	4.75787500	-3.03283300	1.79041900
H	5.67960600	-2.10224500	0.59937100
O	-2.94429500	-1.62272800	-0.41529400
C	-3.81616000	-1.07332400	0.31292400
O	-3.65708000	0.03508600	0.88376800
C	-5.11934300	-1.81625100	0.52909700
H	-5.90185200	-1.14316500	0.87354300
H	-4.95568000	-2.58106600	1.29199900
H	-5.42670500	-2.31860400	-0.38722500

TS_{3-1} optimized by M06-2X/BS2
E(M06-2X-SMD/BS2) = -1332.949053 au
H(M06-2X-SMD/BS2) = -1332.597549 au
G(M06-2X-SMD/BS2) = -1332.684357 au

I	0.51231200	-0.92390200	-0.08184500
C	1.83586400	0.50488100	0.62457900

C	3.55706500	2.41190200	1.56271100
C	2.59997600	1.21155300	-0.29297600
C	1.89965600	0.72070100	1.99280700
C	2.77879600	1.68927800	2.45805300
C	3.46956400	2.17606700	0.19515600
H	2.51205500	1.02104100	-1.35348500
H	1.27746100	0.15681200	2.67453800
H	2.84804700	1.87957100	3.52102700
H	4.07752000	2.74388600	-0.49710500
H	4.23618800	3.16920700	1.93316000
O	-1.26538100	0.78046200	1.05326800
C	-2.50519900	0.34778700	0.73562800
C	-5.06944200	-0.63965700	0.10844700
C	-3.33958100	1.04911500	-0.13935900
C	-2.95946500	-0.84764300	1.28917900
C	-4.22475100	-1.32824200	0.97415200
C	-4.60005400	0.55569300	-0.43791100
H	-2.99224000	1.97675900	-0.57723800
H	-2.31429700	-1.38926900	1.97078600
H	-4.56128100	-2.26003300	1.41540500
H	-5.23654700	1.11341500	-1.11695500
C	-6.44559700	-1.14936300	-0.22186400
H	-6.59768400	-2.15206500	0.17739700
H	-6.60483700	-1.18368100	-1.30134100
H	-7.21710100	-0.49965700	0.19820400
O	-0.25604600	1.25809700	-1.65003000
C	-0.22520800	2.44747900	-1.27428000
O	-0.56218900	2.83546100	-0.11348000
C	0.27758900	3.50659900	-2.22894200
H	0.20824900	3.16730100	-3.26003900
H	1.32860000	3.69744000	-1.99475400
H	-0.26921100	4.43862900	-2.09495500
O	1.79529000	-2.43112200	0.11504300
C	2.77760900	-2.54756500	-0.81240600
O	2.92760000	-1.75728900	-1.70142300
C	3.61195500	-3.76187200	-0.55248700
H	4.03343200	-3.70168900	0.45098300
H	2.97887700	-4.64833900	-0.59893400
H	4.40384700	-3.82309300	-1.29311700
H	-1.01045300	1.69542000	0.57424900

TS$_{7\text{-}10}$ optimized by M06-2X/BS2
E(M06-2X-SMD/BS2) = -1103.834554 au
H(M06-2X-SMD/BS2) = -1103.550914 au
G(M06-2X-SMD/BS2) = -1103.62399 au

I	0.03951400	0.55897000	-0.20687000
C	-2.04215200	0.50749900	-0.02797300
C	-4.77969000	0.46916100	0.21360600
C	-2.60259100	0.17011400	1.19622400
C	-2.81713000	0.82935400	-1.13402800

C	-4.19876100	0.80303300	-1.00460500
C	-3.98655700	0.15624000	1.31025600
H	-1.97402600	-0.07897200	2.04150200
H	-2.35298700	1.09231200	-2.07559700
H	-4.82003400	1.04682300	-1.85678300
H	-4.44222800	-0.10263000	2.25733000
H	-5.85803900	0.45432900	0.30849500
O	-1.66541700	-2.57121800	-0.02922300
C	-0.47182300	-2.35892200	0.05505400
C	2.39378800	-2.36338800	-0.16041100
C	0.36231400	-2.86931200	1.14456100
C	0.24214400	-1.53519400	-0.98430600
C	1.69395700	-1.72850900	-1.11381200
C	1.69785500	-2.88313000	1.01525000
H	-0.14110000	-3.30417600	1.99862400
H	-0.31374100	-1.46501700	-1.91465800
H	2.18317200	-1.30658900	-1.98324800
H	2.30862200	-3.31902500	1.79899900
C	3.87487200	-2.55584700	-0.23259200
H	4.12629600	-3.61757600	-0.17780500
H	4.35745700	-2.06758000	0.61797400
H	4.28332900	-2.14207200	-1.15298200
O	2.69117000	1.53213400	-0.18476600
C	2.37163700	2.65239200	0.28652400
O	1.19657200	3.03667700	0.51106900
C	3.50052600	3.63417400	0.57739300
H	3.19786000	4.37603000	1.31448400
H	3.74990100	4.15430000	-0.35099300
H	4.39234100	3.10771000	0.91525500

$TS_{3\text{-}7}$ optimized by M06-2X/BS2
E(M06-2X-SMD/BS2) = -1332.944359 au
H(M06-2X-SMD/BS2) = -1332.592724 au
G(M06-2X-SMD/BS2) = -1332.678334 au

I	0.15879100	-0.88702700	-0.52365300
C	1.09883700	0.17144600	0.99533600
C	2.34914000	1.50424200	3.02742900
C	1.89769500	1.25689900	0.67320200
C	0.90231900	-0.27275700	2.29462300
C	1.54596400	0.40755700	3.31807700
C	2.52541100	1.92630400	1.71510000
H	2.00928000	1.57486800	-0.35295100
H	0.26345800	-1.12090500	2.50324700
H	1.41307900	0.08176800	4.34142300
H	3.15268000	2.78062900	1.49622800
H	2.84162700	2.03535800	3.83205700
O	-1.48013300	1.98476400	1.24292100
C	-2.09079800	0.88280800	0.83558100
C	-3.47237600	-1.47881700	0.07434900
C	-2.40295000	0.62634500	-0.51127500

C	-2.45716300	-0.08498400	1.79203000
C	-3.12598600	-1.22828800	1.41331200
C	-3.10850200	-0.53166800	-0.86514800
H	-2.14583400	1.36033300	-1.26238100
H	-2.21091000	0.09881300	2.83084500
H	-3.39942600	-1.95528800	2.17098100
H	-3.35860100	-0.68887800	-1.90864300
C	-4.21619500	-2.72986700	-0.29991800
H	-3.64780700	-3.62151700	-0.02661700
H	-4.40893100	-2.76418800	-1.37186400
H	-5.17440900	-2.78574500	0.22114700
O	0.15164100	1.93885700	-1.74316600
C	-0.14793500	3.12990200	-1.54974600
O	-0.79624700	3.56456100	-0.54813500
C	0.28504400	4.17821600	-2.55798200
H	0.71509200	3.71909600	-3.44513800
H	1.02921000	4.82778800	-2.09224900
H	-0.56532600	4.80195000	-2.83492600
O	1.51437200	-2.35761200	-0.48651400
C	2.72691800	-2.10175400	-1.03387800
O	3.01449800	-1.03962700	-1.51006500
C	3.61620800	-3.30219100	-0.93927200
H	3.76219500	-3.55546500	0.11124600
H	3.13591500	-4.15016700	-1.42701500
H	4.56998400	-3.08228300	-1.40983000
H	-1.18403500	2.60836400	0.44677700